Propoxyphene

Other names:	Benzeneethanol, «alpha»-[2-(dimethylamino)-1-methylethyl]-«alpha»-phenyl-, propanoate (ester), [S-(R*,S*)]- 2-Butanol, 4-(dimethylamino)-3-methyl-1,2-diphenyl-, propionate (ester), (2S,3R)- D-propoxyphene Algafan Antalvic Depromic Dextropropoxyphene Benzeneethanol, «alpha»-[2-(dimethylamino)-1-methylethyl]-«alpha»-phenyl-, propanoate, [S-(R*,S*)]- 2-Butanol, 4-(dimethylamino)-3-methyl-1,2-diphenyl-, propionate, (+)- Dextroproxifeno «alpha»-(+)-4-Dimethylamino-1,2-diphenyl-3-methyl-2-butanol propionate ester Propoxyphene, (+)- Proxagesic SK 65 (+)-4-(Dimethylamino)-3-methyl-1,2-diphenyl-2-butanol propionate (2S,3R)-(+)-4-(Dimethylamino)-3-methyl-1,2-diphenyl-2-butanol propionate(ester) «alpha»-d-Propoxyphene Dextropropoxyphen Femadol Darvon
Inchi:	InChI=1S/C22H29NO2/c1-5-21(24)25-22(18(2)17-23(3)4,20-14-10-7-11-15-20)16-19-12-
InchiKey:	XLMALTXPSGQGBX-PGRDOPGGSA-N
Formula:	C22H29NO2
SMILES:	CCC(=O)OC(Cc1ccccc1)(c1ccccc1)C(C)CN(C)C
Mol. weight [g/mol]:	339.47
CAS:	469-62-5

Physical Properties

Property code	Value	Unit	Source
gf	236.44	kJ/mol	Joback Method
hf	-215.65	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	78.63	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.276		Crippen Method
mcvol	290.740	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method

rinpol	2210.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2183.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2203.00		NIST Webbook
rinpol	2229.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2192.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2167.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	841.18	K	Joback Method
tc	1064.91	K	Joback Method
tf	482.59	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.37	J/mol×K	841.18	Joback Method
cpg	916.02	J/mol×K	878.47	Joback Method
cpg	932.33	J/mol×K	915.76	Joback Method
cpg	947.42	J/mol×K	953.04	Joback Method
cpg	961.38	J/mol×K	990.33	Joback Method
cpg	974.34	J/mol×K	1027.62	Joback Method
cpg	986.39	J/mol×K	1064.91	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C469625&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume