2-Butanol, 1,2-diphenyl-4-(methylamino)-3-methyl-, propionate

Other names: 1,2-Diphenyl-4-(methylamino)-3-methyl-2-butanol propionate
Norpropoxyphene
Norpropoxyphene #1
Norpropoxyphene #2

Inchi: InChI=1S/C21H27NO2/c1-4-20(23)24-21(17(2)16-22-3,19-13-9-6-10-14-19)15-18-11-7-5

InchiKey: IKACRWYHQXOSGM-UHFFFAOYSA-N

Formula: C21H27NO2

SMILES: CCC(=O)OC(Cc1ccccc1)(c1ccccc1)C(C)CNC

Mol. weight [g/mol]: 325.44

CAS: 66796-40-5

Physical Properties

Property code	Value	Unit	Source
gf	206.63	kJ/mol	Joback Method
hf	-209.07	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	80.80	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.933		Crippen Method
mcvol	276.650	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2407.00		NIST Webbook
rinpol	2394.00		NIST Webbook
rinpol	2364.00		NIST Webbook
rinpol	2388.00		NIST Webbook
tb	856.03	K	Joback Method
tc	1084.38	K	Joback Method
tf	491.51	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.21	J/mol×K	856.03	Joback Method
cpg	872.71	J/mol×K	894.09	Joback Method
cpg	887.91	J/mol×K	932.15	Joback Method
cpg	901.91	J/mol×K	970.21	Joback Method
cpg	914.82	J/mol×K	1008.27	Joback Method
cpg	926.72	J/mol×K	1046.32	Joback Method
cpg	937.74	J/mol×K	1084.38	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C66796405&Units=SI

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