Proadifen

Other names:	Acetic acid, propyldiphenyl-, 2-(diethylamino)ethyl ester
	BCTB
	Benzeneacetic acid, «alpha»-phenyl-«alpha»-propyl-, 2-(diethylamino)ethyl ester
	2-Diethylaminoethyl-2,2-diphenylvalerate
	2-Diethylaminoethyl propyldiphenylacetate
	HL 8727
	Valeric acid, 2,2-diphenyl-, 2-(diethylamino)ethyl ester
	2,2-Diphenylvaleric acid 2-(diethylamino)ethyl ester
	AV 54315
	Ethyl aprofen
	SKF-525-A
	SK-525-A
Inchi:	InChI=1S/C23H31NO2/c1-4-17-23(20-13-9-7-10-14-20,21-15-11-8-12-16-21)22(25)26-19
InchiKey:	SNTQPLDRUZOSDP-UHFFFAOYSA-N
Formula:	C23H31NO2
SMILES:	CCCC(C(=O)OCCN(CC)CC)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	353.50
CAS:	302-33-0

Physical Properties

Property code	Value	Unit	Source
gf	247.30	kJ/mol	Joback Method
hf	-231.01	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	81.25	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.658		Crippen Method
mcvol	304.830	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinpol	2326.00		NIST Webbook
rinpol	2326.00		NIST Webbook
tb	864.50	K	Joback Method
tc	1083.58	K	Joback Method
tf	508.86	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.10	J/mol×K	864.50	Joback Method
cpg	974.57	J/mol×K	901.01	Joback Method
cpg	990.78	J/mol×K	937.53	Joback Method
cpg	1005.83	J/mol×K	974.04	Joback Method
cpg	1019.83	J/mol×K	1010.55	Joback Method
cpg	1032.87	J/mol×K	1047.07	Joback Method
cpg	1045.07	J/mol×K	1083.58	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=C302330&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