

Sarcosine, N-(1-naphthoyl)-, propyl ester

Inchi:	InChI=1S/C17H19NO3/c1-3-11-21-16(19)12-18(2)17(20)15-10-6-8-13-7-4-5-9-14(13)15/
InchiKey:	KPFUTBYCLGRDIM-UHFFFAOYSA-N
Formula:	C17H19NO3
SMILES:	CCCOC(=O)CN(C)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	285.34

Physical Properties

Property code	Value	Unit	Source
gf	49.63	kJ/mol	Joback Method
hf	-267.93	kJ/mol	Joback Method
hfus	37.86	kJ/mol	Joback Method
hvap	75.96	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	2.865		Crippen Method
mvol	226.160	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook
tb	781.60	K	Joback Method
tc	999.98	K	Joback Method
tf	507.55	K	Joback Method
vc	0.850	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.94	J/molxK	781.60	Joback Method
cpg	661.20	J/molxK	818.00	Joback Method
cpg	674.43	J/molxK	854.39	Joback Method
cpg	686.72	J/molxK	890.79	Joback Method
cpg	698.13	J/molxK	927.19	Joback Method
cpg	708.73	J/molxK	963.59	Joback Method
cpg	718.59	J/molxK	999.98	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=U321399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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