

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

Inchi: InChI=1S/C16H17NO3/c1-3-20-15(18)11-17(2)16(19)14-10-6-8-12-7-4-5-9-13(12)14/h4-16
InchiKey: BWXLOQQWFADZBC-UHFFFAOYSA-N
Formula: C16H17NO3
SMILES: CCOC(=O)CN(C)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 271.31

Physical Properties

Property code	Value	Unit	Source
gf	41.21	kJ/mol	Joback Method
hf	-247.29	kJ/mol	Joback Method
hfus	35.27	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.475		Crippen Method
mcvol	212.070	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	2316.00		NIST Webbook
tb	758.72	K	Joback Method
tc	980.05	K	Joback Method
tf	496.28	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.38	J/mol×K	758.72	Joback Method
cpg	606.32	J/mol×K	795.61	Joback Method
cpg	619.25	J/mol×K	832.50	Joback Method
cpg	631.22	J/mol×K	869.39	Joback Method
cpg	642.32	J/mol×K	906.27	Joback Method
cpg	652.60	J/mol×K	943.16	Joback Method
cpg	662.13	J/mol×K	980.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U321398&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

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