

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

Inchi:	InChI=1S/C18H21NO3/c1-3-4-12-22-17(20)13-19(2)18(21)16-11-7-9-14-8-5-6-10-15(14)
InchiKey:	TULXTVNLKGEGLJ-UHFFFAOYSA-N
Formula:	C18H21NO3
SMILES:	CCCCOC(=O)CN(C)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	299.36

Physical Properties

Property code	Value	Unit	Source
gf	58.05	kJ/mol	Joback Method
hf	-288.57	kJ/mol	Joback Method
hfus	40.45	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.255		Crippen Method
mcvol	240.250	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	2522.00		NIST Webbook
tb	804.48	K	Joback Method
tc	1020.46	K	Joback Method
tf	518.82	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.53	J/molxK	804.48	Joback Method
cpg	717.06	J/molxK	840.48	Joback Method
cpg	730.58	J/molxK	876.47	Joback Method
cpg	743.14	J/molxK	912.47	Joback Method
cpg	754.84	J/molxK	948.47	Joback Method
cpg	765.72	J/molxK	984.47	Joback Method
cpg	775.87	J/molxK	1020.46	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=U321401&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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