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

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

Physical Properties

Property code	Value	Unit	Source
gf	55.61	kJ/mol	Joback Method
hf	-293.85	kJ/mol	Joback Method
hfus	36.93	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.111		Crippen Method
mcvol	240.250	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2465.00		NIST Webbook
tb	804.04	K	Joback Method
tc	1023.17	K	Joback Method
tf	503.82	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.10	J/mol×K	804.04	Joback Method
cpg	717.83	J/mol×K	840.56	Joback Method
cpg	731.51	J/mol×K	877.08	Joback Method
cpg	744.20	J/mol×K	913.61	Joback Method
cpg	755.98	J/mol×K	950.13	Joback Method
cpg	766.92	J/mol×K	986.65	Joback Method
cpg	777.09	J/mol×K	1023.17	Joback Method

Sources

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=U321400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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