Sarcosine, N-hexanoyl-, butyl ester

Inchi: InChI=1S/C13H25NO3/c1-4-6-8-9-12(15)14(3)11-13(16)17-10-7-5-2/h4-11H2,1-3H3
InchiKey: MJGCSNIONZRIJI-UHFFFAOYSA-N
Formula: C13H25NO3
SMILES: CCCCCC(=O)N(C)CC(=O)OCCCC
Mol. weight [g/mol]: 243.35

Physical Properties

Property code	Value	Unit	Source
af	0.7625		Cheméo Relay (1.0)
hf	-717.27	kJ/mol	Cheméo Relay (1.0)
hfus	36.83	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-2.01		Cheméo Relay (1.0)
logp	2.368		Crippen Method
mcvol	213.020	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
tb	557.83	K	Cheméo Relay (1.0)
tc	735.45	K	Cheméo Relay (1.0)
tf	254.72	K	Cheméo Relay (1.0)
vc	0.812	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.23	J/mol×K	639.44	Joback Method
cpg	594.88	J/mol×K	668.69	Joback Method
cpg	609.79	J/mol×K	697.94	Joback Method
cpg	623.98	J/mol×K	727.18	Joback Method
cpg	637.47	J/mol×K	756.43	Joback Method
cpg	650.27	J/mol×K	785.68	Joback Method
cpg	662.39	J/mol×K	814.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321124&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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