Sarcosine, N-isobutyryl-, butyl ester

Inchi: InChI=1S/C11H21NO3/c1-5-6-7-15-10(13)8-12(4)11(14)9(2)3/h9H,5-8H2,1-4H3
InchiKey: YLJPFXZUTLXGHS-UHFFFAOYSA-N
Formula: C11H21NO3
SMILES: CCCCOC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 215.29

Physical Properties

Property code	Value	Unit	Source
gf	-212.76	kJ/mol	Joback Method
hf	-565.50	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.444		Crippen Method
mcvol	184.840	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	593.24	K	Joback Method
tc	774.01	K	Joback Method
tf	353.29	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.99	J/mol×K	593.24	Joback Method
cpg	490.85	J/mol×K	623.37	Joback Method
cpg	505.00	J/mol×K	653.50	Joback Method
cpg	518.47	J/mol×K	683.62	Joback Method
cpg	531.26	J/mol×K	713.75	Joback Method
cpg	543.40	J/mol×K	743.88	Joback Method
cpg	554.90	J/mol×K	774.01	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=U321273&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