Sarcosine, N-isobutyryl-, ethyl ester

Inchi: InChI=1S/C9H17NO3/c1-5-13-8(11)6-10(4)9(12)7(2)3/h7H,5-6H2,1-4H3
InchiKey: ZMUZUZYDOVYEIE-UHFFFAOYSA-N
Formula: C9H17NO3
SMILES: CCOC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 187.24

Physical Properties

Property code	Value	Unit	Source
gf	-229.60	kJ/mol	Joback Method
hf	-524.22	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	53.19	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.664		Crippen Method
mcvol	156.660	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1371.00		NIST Webbook
tb	547.48	K	Joback Method
tc	731.87	K	Joback Method
tf	330.75	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.56	J/mol×K	547.48	Joback Method
cpg	392.05	J/mol×K	578.21	Joback Method
cpg	404.91	J/mol×K	608.94	Joback Method
cpg	417.16	J/mol×K	639.67	Joback Method
cpg	428.81	J/mol×K	670.41	Joback Method
cpg	439.87	J/mol×K	701.14	Joback Method
cpg	450.35	J/mol×K	731.87	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=U321270&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