Sarcosine, N-isobutyryl-, isobutyl ester

Inchi: InChI=1S/C11H21NO3/c1-8(2)7-15-10(13)6-12(5)11(14)9(3)4/h8-9H,6-7H2,1-5H3
InchiKey: ACCHSXWUOMXEOH-UHFFFAOYSA-N
Formula: C11H21NO3
SMILES: CC(C)COC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 215.29

Physical Properties

Property code	Value	Unit	Source
gf	-215.20	kJ/mol	Joback Method
hf	-570.78	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	57.25	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	1.300		Crippen Method
mcvol	184.840	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1516.00		NIST Webbook
rinpol	1516.00		NIST Webbook
tb	592.80	K	Joback Method
tc	776.81	K	Joback Method
tf	338.29	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.37	J/mol×K	592.80	Joback Method
cpg	491.54	J/mol×K	623.47	Joback Method
cpg	505.97	J/mol×K	654.14	Joback Method
cpg	519.69	J/mol×K	684.80	Joback Method
cpg	532.71	J/mol×K	715.47	Joback Method
cpg	545.03	J/mol×K	746.14	Joback Method
cpg	556.68	J/mol×K	776.81	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=U321272&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