Sarcosine, N-(3-methylbut-2-enoyl)-, isohexyl ester

Inchi: InChI=1S/C14H25NO3/c1-11(2)7-6-8-18-14(17)10-15(5)13(16)9-12(3)4/h9,11H,6-8,10H2

InchiKey: SVVZZOAXBYMKJW-UHFFFAOYSA-N

Formula: C14H25NO3

SMILES: CC(C)=CC(=O)N(C)CC(=O)OCCCC(C)C

Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-115.83	kJ/mol	Joback Method
hf	-519.99	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	64.35	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.390		Crippen Method
mcvol	222.810	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1856.00		NIST Webbook
tb	665.92	K	Joback Method
tc	851.21	K	Joback Method
tf	368.06	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.61	J/mol×K	665.92	Joback Method
cpg	627.70	J/mol×K	696.80	Joback Method
cpg	642.95	J/mol×K	727.68	Joback Method
cpg	657.39	J/mol×K	758.56	Joback Method
cpg	671.06	J/mol×K	789.45	Joback Method
cpg	683.98	J/mol×K	820.33	Joback Method
cpg	696.18	J/mol×K	851.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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