

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

Inchi:	InChI=1S/C11H19NO3/c1-5-6-15-11(14)8-12(4)10(13)7-9(2)3/h7H,5-6,8H2,1-4H3
InchiKey:	SNCNQPMOIUNNQU-UHFFFAOYSA-N
Formula:	C11H19NO3
SMILES:	CCCOC(=O)CN(C)C(=O)C=C(C)C
Mol. weight [g/mol]:	213.27

Physical Properties

Property code	Value	Unit	Source
gf	-138.65	kJ/mol	Joback Method
hf	-452.79	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.364		Crippen Method
mcvol	180.540	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
tb	597.72	K	Joback Method
tc	784.89	K	Joback Method
tf	349.25	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.42	J/molxK	597.72	Joback Method
cpg	469.69	J/molxK	628.91	Joback Method
cpg	483.24	J/molxK	660.11	Joback Method
cpg	496.08	J/molxK	691.30	Joback Method
cpg	508.25	J/molxK	722.50	Joback Method
cpg	519.76	J/molxK	753.69	Joback Method
cpg	530.65	J/molxK	784.89	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U321519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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