

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

Inchi:	InChI=1S/C10H17NO3/c1-5-14-10(13)7-11(4)9(12)6-8(2)3/h6H,5,7H2,1-4H3
InchiKey:	RNQTUFWNTCTKHH-UHFFFAOYSA-N
Formula:	C10H17NO3
SMILES:	CCOC(=O)CN(C)C(=O)C=C(C)C
Mol. weight [g/mol]:	199.25

Physical Properties

Property code	Value	Unit	Source
gf	-147.07	kJ/mol	Joback Method
hf	-432.15	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	55.84	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.974		Crippen Method
mcvol	166.450	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook
tb	574.84	K	Joback Method
tc	764.12	K	Joback Method
tf	337.98	K	Joback Method
vc	0.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.49	J/mol×K	574.84	Joback Method
cpg	420.11	J/mol×K	606.39	Joback Method
cpg	433.04	J/mol×K	637.93	Joback Method
cpg	445.29	J/mol×K	669.48	Joback Method
cpg	456.89	J/mol×K	701.03	Joback Method
cpg	467.87	J/mol×K	732.57	Joback Method
cpg	478.24	J/mol×K	764.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U321518&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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