

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

Inchi:	InChI=1S/C17H31NO3/c1-5-6-7-8-9-10-11-12-21-17(20)14-18(4)16(19)13-15(2)3/h13H,5
InchiKey:	LALRZVXAFXNUSH-UHFFFAOYSA-N
Formula:	C17H31NO3
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)C=C(C)C
Mol. weight [g/mol]:	297.43

Physical Properties

Property code	Value	Unit	Source
gf	-88.13	kJ/mol	Joback Method
hf	-576.63	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	71.42	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.705		Crippen Method
mcvol	265.080	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	735.00	K	Joback Method
tc	916.46	K	Joback Method
tf	416.87	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.46	J/mol×K	735.00	Joback Method
cpg	795.46	J/mol×K	765.24	Joback Method
cpg	811.58	J/mol×K	795.49	Joback Method
cpg	826.85	J/mol×K	825.73	Joback Method
cpg	841.31	J/mol×K	855.98	Joback Method
cpg	855.00	J/mol×K	886.22	Joback Method
cpg	867.94	J/mol×K	916.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321521&Units=SI
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

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

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