

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

Inchi: InChI=1S/C20H37NO3/c1-5-6-7-8-9-10-11-12-13-14-15-24-20(23)17-21(4)19(22)16-18(2)
InchiKey: ATNQMUUQFMEQGU-UHFFFAOYSA-N
Formula: C20H37NO3
SMILES: CCCCCCCCCCCCCOC(=O)CN(C)C(=O)C=C(C)C
Mol. weight [g/mol]: 339.51

Physical Properties

Property code	Value	Unit	Source
gf	-62.87	kJ/mol	Joback Method
hf	-638.55	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	78.10	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.875		Crippen Method
mcvol	307.350	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	803.64	K	Joback Method
tc	989.00	K	Joback Method
tf	450.68	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.21	J/mol×K	803.64	Joback Method
cpg	973.35	J/mol×K	834.53	Joback Method
cpg	990.50	J/mol×K	865.43	Joback Method
cpg	1006.72	J/mol×K	896.32	Joback Method
cpg	1022.04	J/mol×K	927.21	Joback Method
cpg	1036.51	J/mol×K	958.10	Joback Method
cpg	1050.18	J/mol×K	989.00	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=U321523&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
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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