

Sarcosine, N-valeryl-, dodecyl ester

Inchi:	InChI=1S/C20H39NO3/c1-4-6-8-9-10-11-12-13-14-15-17-24-20(23)18-21(3)19(22)16-7-5
InchiKey:	AATJXMIVDDBCNG-UHFFFAOYSA-N
Formula:	C20H39NO3
SMILES:	CCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCC
Mol. weight [g/mol]:	341.53

Physical Properties

Property code	Value	Unit	Source
gf	-134.54	kJ/mol	Joback Method
hf	-745.98	kJ/mol	Joback Method
hfus	54.96	kJ/mol	Joback Method
hvap	78.06	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.099		Crippen Method
mvol	311.650	ml/mol	McGowan Method
pc	1088.50	kPa	Joback Method
rinpol	2514.00		NIST Webbook
tb	799.60	K	Joback Method
tc	981.59	K	Joback Method
tf	469.72	K	Joback Method
vc	1.204	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.61	J/mol×K	799.60	Joback Method
cpg	999.23	J/mol×K	829.93	Joback Method
cpg	1016.83	J/mol×K	860.26	Joback Method
cpg	1033.45	J/mol×K	890.59	Joback Method
cpg	1049.12	J/mol×K	920.93	Joback Method
cpg	1063.86	J/mol×K	951.26	Joback Method
cpg	1077.72	J/mol×K	981.59	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=U321567&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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