

Sarcosine, n-heptafluorobutyryl-, ethyl ester

Inchi:	InChI=1S/C9H10F7NO3/c1-3-20-5(18)4-17(2)6(19)7(10,11)8(12,13)9(14,15)16/h3-4H2,1
InchiKey:	RUOVTXQTMRODG-UHFFFAOYSA-N
Formula:	C9H10F7NO3
SMILES:	CCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	313.17

Physical Properties

Property code	Value	Unit	Source
gf	-1582.31	kJ/mol	Joback Method
hf	-1917.96	kJ/mol	Joback Method
hfus	25.79	kJ/mol	Joback Method
hvap	43.97	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.841		Crippen Method
mcvol	169.050	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	980.00		NIST Webbook
tb	533.12	K	Joback Method
tc	689.56	K	Joback Method
tf	357.14	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.51	J/molxK	533.12	Joback Method
cpg	457.18	J/molxK	559.19	Joback Method
cpg	468.13	J/molxK	585.27	Joback Method
cpg	478.39	J/molxK	611.34	Joback Method
cpg	488.00	J/molxK	637.42	Joback Method
cpg	496.99	J/molxK	663.49	Joback Method
cpg	505.38	J/molxK	689.56	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=U321254&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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