

Sarcosine, n-heptafluorobutyryl-, butyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C11H14F7NO3/c1-3-4-5-22-7(20)6-19(2)8(21)9(12,13)10(14,15)11(16,17)18/h

CXBXPQYSYFOJMR-UHFFFAOYSA-N

C11H14F7NO3

CCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F

341.22

Physical Properties

Property code	Value	Unit	Source
gf	-1565.47	kJ/mol	Joback Method
hf	-1959.24	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	48.42	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.621		Crippen Method
mcvol	197.230	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	1321.00		NIST Webbook
rinpol	1321.00		NIST Webbook
tb	578.88	K	Joback Method
tc	735.09	K	Joback Method
tf	379.68	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.84	J/mol×K	578.88	Joback Method
cpg	554.50	J/mol×K	604.91	Joback Method
cpg	566.41	J/mol×K	630.95	Joback Method
cpg	577.60	J/mol×K	656.98	Joback Method
cpg	588.11	J/mol×K	683.02	Joback Method
cpg	597.98	J/mol×K	709.05	Joback Method
cpg	607.25	J/mol×K	735.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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