

Sarcosine, N-heptafluorobutyryl-, heptyl ester

Inchi:	InChI=1S/C14H20F7NO3/c1-3-4-5-6-7-8-25-10(23)9-22(2)11(24)12(15,16)13(17,18)14(19)21
InchiKey:	UTHMOGRSMJPFQD-UHFFFAOYSA-N
Formula:	C14H20F7NO3
SMILES:	CCCCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	383.30

Physical Properties

Property code	Value	Unit	Source
hfus	38.74	kJ/mol	Joback Method
hvap	74.85	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.78		Cheméo Relay (1.0)
logp	3.791		Crippen Method
mcvol	239.500	ml/mol	McGowan Method
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
tb	519.47	K	Cheméo Relay (1.0)
tf	248.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.69	J/mol×K	647.52	Joback Method
cpg	710.64	J/mol×K	673.88	Joback Method
cpg	723.79	J/mol×K	700.24	Joback Method
cpg	736.18	J/mol×K	726.60	Joback Method
cpg	747.85	J/mol×K	752.96	Joback Method
cpg	758.85	J/mol×K	779.32	Joback Method
cpg	769.22	J/mol×K	805.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321260&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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