

Sarcosine, n-heptafluorobutyryl-, isobutyl ester

Inchi:	InChI=1S/C11H14F7NO3/c1-6(2)5-22-7(20)4-19(3)8(21)9(12,13)10(14,15)11(16,17)18/h
InchiKey:	WZIYWGOTWAWROP-UHFFFAOYSA-N
Formula:	C11H14F7NO3
SMILES:	CC(C)COC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	341.22

Physical Properties

Property code	Value	Unit	Source
gf	-1567.91	kJ/mol	Joback Method
hf	-1964.52	kJ/mol	Joback Method
hfus	27.45	kJ/mol	Joback Method
hvap	48.03	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.477		Crippen Method
mcvol	197.230	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	1286.00		NIST Webbook
tb	578.44	K	Joback Method
tc	736.92	K	Joback Method
tf	364.68	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.20	J/mol×K	578.44	Joback Method
cpg	555.09	J/mol×K	604.85	Joback Method
cpg	567.20	J/mol×K	631.27	Joback Method
cpg	578.57	J/mol×K	657.68	Joback Method
cpg	589.24	J/mol×K	684.09	Joback Method
cpg	599.24	J/mol×K	710.51	Joback Method
cpg	608.62	J/mol×K	736.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321256&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
hvac:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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