Sarcosine, n-heptafluorobutyryl-, propyl ester

Inchi: InChI=1S/C10H12F7NO3/c1-3-4-21-6(19)5-18(2)7(20)8(11,12)9(13,14)10(15,16)17/h3-5
InchiKey: JAGXIGPBGDVLTE-UHFFFAOYSA-N
Formula: C10H12F7NO3
SMILES: CCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 327.20

Physical Properties

Property code	Value	Unit	Source
gf	-1573.89	kJ/mol	Joback Method
hf	-1938.60	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Joback Method
hvap	46.19	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.231		Crippen Method
mcvol	183.140	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	1229.00		NIST Webbook
tb	556.00	K	Joback Method
tc	712.21	K	Joback Method
tf	368.41	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.93	J/mol×K	556.00	Joback Method
cpg	505.11	J/mol×K	582.04	Joback Method
cpg	516.56	J/mol×K	608.07	Joback Method
cpg	527.31	J/mol×K	634.11	Joback Method
cpg	537.39	J/mol×K	660.14	Joback Method
cpg	546.83	J/mol×K	686.18	Joback Method
cpg	555.68	J/mol×K	712.21	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=U321255&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/75-553-5/Sarcosine-n-heptafluorobutyryl-propyl-ester.pdf
Generated by Cheméo on 2024-04-25 09:12:36.089711066 +0000 UTC m=+16325605.010288393.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.