Sarcosine, N-heptafluorobutyryl-, pentadecyl ester

Inchi: InChI=1S/C22H36F7NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-33-18(31)17-30(2)19(3

InchiKey: DYGVBQDDLBWYDB-UHFFFAOYSA-N

Formula: C22H36F7NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 495.52

Physical Properties

Property code	Value	Unit	Source
hfus	59.46	kJ/mol	Joback Method
hvap	107.46	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.29		Cheméo Relay (1.0)
logp	6.912		Crippen Method
mcvol	352.220	ml/mol	McGowan Method
rinpol	2346.00		NIST Webbook
tb	605.33	K	Cheméo Relay (1.0)
tf	285.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.75	J/mol×K	830.56	Joback Method
cpg	1174.83	J/mol×K	861.89	Joback Method
cpg	1191.82	J/mol×K	893.21	Joback Method
cpg	1207.82	J/mol×K	924.54	Joback Method
cpg	1222.91	J/mol×K	955.87	Joback Method
cpg	1237.18	J/mol×K	987.19	Joback Method
cpg	1250.71	J/mol×K	1018.52	Joback Method

Sources

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=U321266&Units=SI
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
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