

Sarcosine, N-heptafluorobutyryl-, octadecyl ester

Inchi: InChI=1S/C25H42F7NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-36-21(34)20.
InchiKey: LGEZHUOBMHLAQZ-UHFFFAOYSA-N
Formula: C25H42F7NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 537.60

Physical Properties

Property code	Value	Unit	Source
hfus	67.23	kJ/mol	Joback Method
hvap	118.79	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.08		Cheméo Relay (1.0)
logp	8.082		Crippen Method
mcvol	394.490	ml/mol	McGowan Method
rinpol	2629.00		NIST Webbook
rinpol	2629.00		NIST Webbook
tb	630.85	K	Cheméo Relay (1.0)
tf	295.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1342.50	J/mol×K	899.20	Joback Method
cpg	1363.10	J/mol×K	934.79	Joback Method
cpg	1382.40	J/mol×K	970.39	Joback Method
cpg	1400.54	J/mol×K	1005.98	Joback Method
cpg	1417.65	J/mol×K	1041.57	Joback Method
cpg	1433.88	J/mol×K	1077.16	Joback Method
cpg	1449.36	J/mol×K	1112.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321269&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

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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