

«beta»-Alanine, n-heptafluorobutyryl-, tetradecyl ester

Inchi: InChI=1S/C21H34F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-32-17(30)14-15-29-18(31)19-20
InchiKey: HZXRIAXXRDQPLP-UHFFFAOYSA-N
Formula: C21H34F7NO3
SMILES: CCCCCCCCCCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 481.49

Physical Properties

Property code	Value	Unit	Source
gf	-1502.66	kJ/mol	Joback Method
hf	-2179.70	kJ/mol	Joback Method
hfus	58.95	kJ/mol	Joback Method
hvap	75.07	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.570		Crippen Method
mcvol	338.130	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	845.41	K	Joback Method
tc	1036.59	K	Joback Method
tf	512.57	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.37	J/mol×K	845.41	Joback Method
cpg	1133.42	J/mol×K	877.27	Joback Method
cpg	1149.42	J/mol×K	909.14	Joback Method
cpg	1164.46	J/mol×K	941.00	Joback Method
cpg	1178.63	J/mol×K	972.86	Joback Method
cpg	1192.00	J/mol×K	1004.73	Joback Method
cpg	1204.67	J/mol×K	1036.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinsol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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