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

Inchi: InChI=1S/C20H34F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-29-17(27)14-15-26-18(28)1

InchiKey: FJGQICFQMHGYNW-UHFFFAOYSA-N

Formula: C20H34F5NO3

SMILES: CCCCCCCCCCCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 431.48

Physical Properties

Property code	Value	Unit	Source
gf	-1124.30	kJ/mol	Joback Method
hf	-1758.09	kJ/mol	Joback Method
hfus	57.61	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	5.935		Crippen Method
mcvol	320.500	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinpol	2243.00		NIST Webbook
rinpol	2243.00		NIST Webbook
tb	827.22	K	Joback Method
tc	1012.80	K	Joback Method
tf	497.70	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.62	J/mol×K	827.22	Joback Method
cpg	1057.48	J/mol×K	858.15	Joback Method
cpg	1073.34	J/mol×K	889.08	Joback Method
cpg	1088.25	J/mol×K	920.01	Joback Method
cpg	1102.28	J/mol×K	950.94	Joback Method
cpg	1115.48	J/mol×K	981.87	Joback Method
cpg	1127.92	J/mol×K	1012.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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