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

Inchi: InChI=1S/C24H40F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-35-20(33)17-18-3

InchiKey: OTCKMLPNRZEBQK-UHFFFAOYSA-N

Formula: C24H40F7NO3

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

Mol. weight [g/mol]: 523.57

Physical Properties

Property code	Value	Unit	Source
gf	-1477.40	kJ/mol	Joback Method
hf	-2241.62	kJ/mol	Joback Method
hfus	66.72	kJ/mol	Joback Method
hvap	81.75	kJ/mol	Joback Method
log10ws	-8.99		Crippen Method
logp	7.740		Crippen Method
mcvol	380.400	ml/mol	McGowan Method
pc	747.33	kPa	Joback Method
rinpol	2556.00		NIST Webbook
rinpol	2556.00		NIST Webbook
tb	914.05	K	Joback Method
tc	1130.75	K	Joback Method
tf	546.38	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.49	J/mol×K	914.05	Joback Method
cpg	1319.98	J/mol×K	950.17	Joback Method
cpg	1338.21	J/mol×K	986.28	Joback Method
cpg	1355.32	J/mol×K	1022.40	Joback Method
cpg	1371.44	J/mol×K	1058.51	Joback Method
cpg	1386.70	J/mol×K	1094.63	Joback Method
cpg	1401.24	J/mol×K	1130.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320988&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