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

Inchi: InChI=1S/C25H42F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-36-21(34)18-1

InchiKey: YKTFLMBVZLWKHP-UHFFFAOYSA-N

Formula: C25H42F7NO3

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

Mol. weight [g/mol]: 537.59

Physical Properties

Property code	Value	Unit	Source
gf	-1468.98	kJ/mol	Joback Method
hf	-2262.26	kJ/mol	Joback Method
hfus	69.31	kJ/mol	Joback Method
hvap	83.97	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	8.130		Crippen Method
mcvol	394.490	ml/mol	McGowan Method
pc	709.60	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	936.93	K	Joback Method
tc	1164.57	K	Joback Method
tf	557.65	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.12	J/mol×K	936.93	Joback Method
cpg	1383.61	J/mol×K	974.87	Joback Method
cpg	1402.75	J/mol×K	1012.81	Joback Method
cpg	1420.71	J/mol×K	1050.75	Joback Method
cpg	1437.64	J/mol×K	1088.69	Joback Method
cpg	1453.70	J/mol×K	1126.63	Joback Method
cpg	1469.05	J/mol×K	1164.57	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320989&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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