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

Inchi: InChI=1S/C19H30F7NO3/c1-2-3-4-5-6-7-8-9-10-11-14-30-15(28)12-13-27-16(29)17(20,2

InchiKey: GMOYZXQSNFWOMT-UHFFFAOYSA-N

Formula: C19H30F7NO3

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

Mol. weight [g/mol]: 453.44

Physical Properties

Property code	Value	Unit	Source
gf	-1519.50	kJ/mol	Joback Method
hf	-2138.42	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.790		Crippen Method
mcvol	309.950	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	799.65	K	Joback Method
tc	979.00	K	Joback Method
tf	490.03	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.18	J/mol×K	799.65	Joback Method
cpg	1012.95	J/mol×K	829.54	Joback Method
cpg	1027.79	J/mol×K	859.43	Joback Method
cpg	1041.74	J/mol×K	889.33	Joback Method
cpg	1054.89	J/mol×K	919.22	Joback Method
cpg	1067.30	J/mol×K	949.11	Joback Method
cpg	1079.02	J/mol×K	979.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320984&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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