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

Inchi: InChI=1S/C21H36F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-30-18(28)15-16-27-19(2

InchiKey: NCUDISXZNIRXST-UHFFFAOYSA-N

Formula: C21H36F5NO3

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

Mol. weight [g/mol]: 445.51

Physical Properties

Property code	Value	Unit	Source
gf	-1115.88	kJ/mol	Joback Method
hf	-1778.73	kJ/mol	Joback Method
hfus	60.20	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.325		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	850.10	K	Joback Method
tc	1041.57	K	Joback Method
tf	508.97	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.04	J/mol×K	850.10	Joback Method
cpg	1118.53	J/mol×K	882.01	Joback Method
cpg	1134.95	J/mol×K	913.92	Joback Method
cpg	1150.37	J/mol×K	945.84	Joback Method
cpg	1164.86	J/mol×K	977.75	Joback Method
cpg	1178.49	J/mol×K	1009.66	Joback Method
cpg	1191.33	J/mol×K	1041.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320959&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