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

Inchi: InChI=1S/C16H26F5NO3/c1-2-3-4-5-6-7-8-9-12-25-13(23)10-11-22-14(24)15(17,18)16(1

InchiKey: WYJGCVHNNHDVBT-UHFFFAOYSA-N

Formula: C16H26F5NO3

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

Mol. weight [g/mol]: 375.37

Physical Properties

Property code	Value	Unit	Source
gf	-1157.98	kJ/mol	Joback Method
hf	-1675.53	kJ/mol	Joback Method
hfus	47.25	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.374		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
tb	735.70	K	Joback Method
tc	906.03	K	Joback Method
tf	452.62	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.17	J/mol×K	735.70	Joback Method
cpg	821.93	J/mol×K	764.09	Joback Method
cpg	835.87	J/mol×K	792.48	Joback Method
cpg	849.03	J/mol×K	820.87	Joback Method
cpg	861.44	J/mol×K	849.25	Joback Method
cpg	873.15	J/mol×K	877.64	Joback Method
cpg	884.19	J/mol×K	906.03	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=U320955&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