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

Inchi: InChI=1S/C15H24F5NO3/c1-2-3-4-5-6-7-8-11-24-12(22)9-10-21-13(23)14(16,17)15(18,1

InchiKey: BLFGOOAXXPPXMS-UHFFFAOYSA-N

Formula: C15H24F5NO3

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

Mol. weight [g/mol]: 361.35

Physical Properties

Property code	Value	Unit	Source
gf	-1166.40	kJ/mol	Joback Method
hf	-1654.89	kJ/mol	Joback Method
hfus	44.66	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.984		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	712.82	K	Joback Method
tc	881.08	K	Joback Method
tf	441.35	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.17	J/mol×K	712.82	Joback Method
cpg	765.47	J/mol×K	740.86	Joback Method
cpg	778.97	J/mol×K	768.91	Joback Method
cpg	791.72	J/mol×K	796.95	Joback Method
cpg	803.76	J/mol×K	825.00	Joback Method
cpg	815.11	J/mol×K	853.04	Joback Method
cpg	825.82	J/mol×K	881.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320954&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