.beta.-Alanine, N-pentafluoropropionyl-, dodecyl ester

Inchi: InChI=1S/C18H30F5NO3/c1-2-3-4-5-6-7-8-9-10-11-14-27-15(25)12-13-24-16(26)17(19,2

InchiKey: XMCBWAAOUREPSF-UHFFFAOYSA-N

Formula: C18H30F5NO3

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

Mol. weight [g/mol]: 403.43

Physical Properties

Property code	Value	Unit	Source
hf	-1889.74	kJ/mol	Cheméo Relay (1.0)
hfus	52.43	kJ/mol	Joback Method
hvap	97.11	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.97		Cheméo Relay (1.0)
logp	5.154		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	579.98	K	Cheméo Relay (1.0)
tc	719.26	K	Cheméo Relay (1.0)
tf	316.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.13	J/mol×K	781.46	Joback Method
cpg	937.88	J/mol×K	810.86	Joback Method
cpg	952.73	J/mol×K	840.27	Joback Method
cpg	966.72	J/mol×K	869.67	Joback Method
cpg	979.90	J/mol×K	899.08	Joback Method
cpg	992.33	J/mol×K	928.48	Joback Method
cpg	1004.05	J/mol×K	957.89	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320957&Units=SI

Legend

cpg:	Ideal gas heat capacity
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