

.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(19,20)21
InchiKey:	WYJGCVHNNHDTVBT-UHFFFAOYSA-N
Formula:	C16H26F5NO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	375.38

Physical Properties

Property code	Value	Unit	Source
hf	-1849.65	kJ/mol	Cheméo Relay (1.0)
hfus	47.25	kJ/mol	Joback Method
hvap	88.94	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.33		Cheméo Relay (1.0)
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	559.46	K	Cheméo Relay (1.0)
tc	698.80	K	Cheméo Relay (1.0)
tf	308.05	K	Cheméo Relay (1.0)

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

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=U320955&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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