.beta.-Alanine, N-heptafluorobutyryl-, undecyl ester

Inchi: InChI=1S/C18H28F7NO3/c1-2-3-4-5-6-7-8-9-10-13-29-14(27)11-12-26-15(28)16(19,20)1

InchiKey: PBPQESVEGHCUJW-UHFFFAOYSA-N

Formula: C18H28F7NO3

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

Mol. weight [g/mol]: 439.41

Physical Properties

Property code	Value	Unit	Source
hf	-2277.12	kJ/mol	Cheméo Relay (1.0)
hfus	51.18	kJ/mol	Joback Method
hvap	95.84	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.39		Cheméo Relay (1.0)
logp	5.400		Crippen Method
mcvol	295.860	ml/mol	McGowan Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	579.22	K	Cheméo Relay (1.0)
tc	707.77	K	Cheméo Relay (1.0)
tf	300.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.79	J/mol×K	776.77	Joback Method
cpg	954.01	J/mol×K	805.90	Joback Method
cpg	968.32	J/mol×K	835.02	Joback Method
cpg	981.80	J/mol×K	864.15	Joback Method
cpg	994.50	J/mol×K	893.27	Joback Method
cpg	1006.47	J/mol×K	922.40	Joback Method
cpg	1017.78	J/mol×K	951.52	Joback Method

Sources

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=U320983&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point