Pentadecafluorooctanoic acid, undecyl ester

Inchi: InChI=1S/C19H23F15O2/c1-2-3-4-5-6-7-8-9-10-11-36-12(35)13(20,21)14(22,23)15(24,25
InchiKey: FVSCXMNVWQIEAW-UHFFFAOYSA-N
Formula: C19H23F15O2
SMILES: CCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 568.36

Physical Properties

Property code	Value	Unit	Source
gf	-3027.09	kJ/mol	Joback Method
hf	-3683.19	kJ/mol	Joback Method
hfus	42.05	kJ/mol	Joback Method
hvap	45.72	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	8.434		Crippen Method
mcvol	312.560	ml/mol	McGowan Method
pc	798.89	kPa	Joback Method
rinpol	1556.00		NIST Webbook
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tb	676.85	K	Joback Method
tc	828.78	K	Joback Method
tf	401.84	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.05	J/mol×K	676.85	Joback Method
cpg	994.68	J/mol×K	702.17	Joback Method
cpg	1009.31	J/mol×K	727.49	Joback Method
cpg	1023.03	J/mol×K	752.82	Joback Method
cpg	1035.90	J/mol×K	778.14	Joback Method
cpg	1047.99	J/mol×K	803.46	Joback Method
cpg	1059.37	J/mol×K	828.78	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=U406041&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