

Pentadecafluorooctanoic acid, naphth-2-yl ester

Inchi: InChI=1S/C18H7F15O2/c19-12(20,11(34)35-10-6-5-8-3-1-2-4-9(8)7-10)13(21,22)14(23,24)15
InchiKey: BTKBLUGSWYMAIB-UHFFFAOYSA-N
Formula: C18H7F15O2
SMILES: O=C(Oc1ccc2ccccc2c1)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)
Mol. weight [g/mol]: 540.22

Physical Properties

Property code	Value	Unit	Source
gf	-2826.08	kJ/mol	Joback Method
hf	-3246.42	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	7.119		Crippen Method
mvol	255.250	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	704.61	K	Joback Method
tc	876.59	K	Joback Method
tf	462.21	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.25	J/molxK	704.61	Joback Method
cpg	791.04	J/molxK	733.27	Joback Method
cpg	800.84	J/molxK	761.94	Joback Method
cpg	809.77	J/molxK	790.60	Joback Method
cpg	817.95	J/molxK	819.26	Joback Method
cpg	825.49	J/molxK	847.92	Joback Method
cpg	832.51	J/molxK	876.59	Joback Method

Sources

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=U406893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/78-260-7/Pentadecafluorooctanoic-acid-naphth-2-yl-ester.pdf>

Generated by Cheméo on 2024-04-26 18:42:34.873594048 +0000 UTC m=+16446203.794171363.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.