Heptadecafluorononanoic acid, heptyl ester

Other names: Heptadecafluorononanoic acid, heptyl ester
Inchi: InChI=1S/C16H15F17O2/c1-2-3-4-5-6-7-35-8(34)9(17,18)10(19,20)11(21,22)12(23,24)13
InchiKey: UKDOQBCXBIOHIG-UHFFFAOYSA-N
Formula: C16H15F17O2
SMILES: CCCCCCCOC(=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)C(F)(F)F
Mol. weight [g/mol]: 562.26

Physical Properties

Property code	Value	Unit	Source
hf	-4061.39	kJ/mol	Cheméo Relay (1.0)
hfus	33.03	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.70		Cheméo Relay (1.0)
logp	7.509		Crippen Method
mcvol	273.830	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	1240.00		NIST Webbook
tb	515.91	K	Cheméo Relay (1.0)
tc	626.65	K	Cheméo Relay (1.0)
tf	294.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.48	J/mol×K	603.52	Joback Method
cpg	845.69	J/mol×K	626.59	Joback Method
cpg	858.95	J/mol×K	649.65	Joback Method
cpg	871.32	J/mol×K	672.72	Joback Method
cpg	882.85	J/mol×K	695.79	Joback Method
cpg	893.60	J/mol×K	718.86	Joback Method
cpg	903.64	J/mol×K	741.92	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=C127392534&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