Heptadecafluorononanoic acid, dodecyl ester

Inchi: InChI=1S/C21H25F17O2/c1-2-3-4-5-6-7-8-9-10-11-12-40-13(39)14(22,23)15(24,25)16(2
InchiKey: JNWYTNPCXKXCEK-UHFFFAOYSA-N
Formula: C21H25F17O2
SMILES: CCCCCCCCCCCCOC(=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]: 632.39

Physical Properties

Property code	Value	Unit	Source
gf	-3397.03	kJ/mol	Joback Method
hf	-4125.44	kJ/mol	Joback Method
hfus	45.98	kJ/mol	Joback Method
hvap	47.24	kJ/mol	Joback Method
log10ws	-10.34		Crippen Method
logp	9.460		Crippen Method
mcvol	344.280	ml/mol	McGowan Method
pc	692.16	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tb	717.92	K	Joback Method
tc	880.38	K	Joback Method
tf	427.98	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1111.47	J/mol×K	717.92	Joback Method
cpg	1127.89	J/mol×K	745.00	Joback Method
cpg	1143.20	J/mol×K	772.07	Joback Method
cpg	1157.51	J/mol×K	799.15	Joback Method
cpg	1170.92	J/mol×K	826.23	Joback Method
cpg	1183.52	J/mol×K	853.30	Joback Method
cpg	1195.43	J/mol×K	880.38	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=U356028&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