Pentadecafluorooctanoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H7F15O2/c1-6-3-2-4-7(5-6)32-8(31)9(16,17)10(18,19)11(20,21)12(22,23)1
InchiKey: LNYMAXSBBHLYDT-UHFFFAOYSA-N
Formula: C15H7F15O2
SMILES: Cc1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 504.19

Physical Properties

Property code	Value	Unit	Source
gf	-2957.99	kJ/mol	Joback Method
hf	-3375.57	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	39.75	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.275		Crippen Method
mcvol	232.440	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	1218.00		NIST Webbook
rinpol	1218.00		NIST Webbook
tb	616.99	K	Joback Method
tc	773.62	K	Joback Method
tf	395.70	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.37	J/mol×K	616.99	Joback Method
cpg	699.52	J/mol×K	643.09	Joback Method
cpg	710.65	J/mol×K	669.20	Joback Method
cpg	720.85	J/mol×K	695.30	Joback Method
cpg	730.19	J/mol×K	721.41	Joback Method
cpg	738.73	J/mol×K	747.51	Joback Method
cpg	746.56	J/mol×K	773.62	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=U406891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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