Phloroglucinol, tris(pentafluoropropionate)

Inchi: InChI=1S/C15H3F15O6/c16-10(17,13(22,23)24)7(31)34-4-1-5(35-8(32)11(18,19)14(25,2
InchiKey: SFUNGGZHAOPZID-UHFFFAOYSA-N
Formula: C15H3F15O6
SMILES: O=C(Oc1cc(OC(=O)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)F)c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 564.16

Physical Properties

Property code	Value	Unit	Source
gf	-3438.30	kJ/mol	Joback Method
hf	-3867.89	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	4.996		Crippen Method
mcvol	247.320	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	1087.00		NIST Webbook
tb	777.78	K	Joback Method
tc	954.47	K	Joback Method
tf	550.12	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.02	J/mol×K	777.78	Joback Method
cpg	769.95	J/mol×K	807.23	Joback Method
cpg	777.11	J/mol×K	836.68	Joback Method
cpg	783.56	J/mol×K	866.13	Joback Method
cpg	789.38	J/mol×K	895.58	Joback Method
cpg	794.65	J/mol×K	925.02	Joback Method
cpg	799.42	J/mol×K	954.47	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=U375765&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

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