Phloroglucinol, tris(heptafluorobutyrate)

Inchi: InChI=1S/C18H3F21O6/c19-10(20,13(25,26)16(31,32)33)7(40)43-4-1-5(44-8(41)11(21,2
InchiKey: SMOFGZJTWDOHDU-UHFFFAOYSA-N
Formula: C18H3F21O6
SMILES: O=C(Oc1cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1)C(F)(
Mol. weight [g/mol]: 714.18

Physical Properties

Property code	Value	Unit	Source
gf	-4573.38	kJ/mol	Joback Method
hf	-5132.72	kJ/mol	Joback Method
hfus	41.95	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	6.902		Crippen Method
mcvol	300.210	ml/mol	McGowan Method
pc	928.94	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
tb	832.35	K	Joback Method
tc	1021.32	K	Joback Method
tf	594.73	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.82	J/mol×K	832.35	Joback Method
cpg	980.76	J/mol×K	863.85	Joback Method
cpg	987.89	J/mol×K	895.34	Joback Method
cpg	994.36	J/mol×K	926.84	Joback Method
cpg	1000.31	J/mol×K	958.33	Joback Method
cpg	1005.87	J/mol×K	989.83	Joback Method
cpg	1011.19	J/mol×K	1021.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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