2-Methylresorcinol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C15H6F14O4/c1-5-6(32-8(30)10(16,17)12(20,21)14(24,25)26)3-2-4-7(5)33-9(3
InchiKey: ADTUSTWHWGNYRH-UHFFFAOYSA-N
Formula: C15H6F14O4
SMILES: Cc1c(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 516.18

Physical Properties

Property code	Value	Unit	Source
gf	-3009.57	kJ/mol	Joback Method
hf	-3426.98	kJ/mol	Joback Method
hfus	32.08	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.472		Crippen Method
mcvol	238.110	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	1181.00		NIST Webbook
rinpol	1181.00		NIST Webbook
tb	702.22	K	Joback Method
tc	869.46	K	Joback Method
tf	477.37	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.75	J/mol×K	702.22	Joback Method
cpg	728.66	J/mol×K	730.09	Joback Method
cpg	737.73	J/mol×K	757.97	Joback Method
cpg	746.03	J/mol×K	785.84	Joback Method
cpg	753.63	J/mol×K	813.72	Joback Method
cpg	760.59	J/mol×K	841.59	Joback Method
cpg	766.98	J/mol×K	869.46	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=U375884&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