Ethylene glycol monosalicylate, bis(pentafluoropropionate)

Inchi: InChI=1S/C15H8F10O6/c16-12(17,14(20,21)22)10(27)30-6-5-29-9(26)7-3-1-2-4-8(7)31-1

InchiKey: NVQZXNITDHYSQM-UHFFFAOYSA-N

Formula: C15H8F10O6

SMILES: O=C(OCCOC(=O)C(F)(F)C(F)(F)F)c1ccccc1OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 474.20

Physical Properties

Property code	Value	Unit	Source
gf	-2460.30	kJ/mol	Joback Method
hf	-2858.37	kJ/mol	Joback Method
hfus	37.76	kJ/mol	Joback Method
hvap	66.04	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.687		Crippen Method
mcvol	238.470	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
tb	782.91	K	Joback Method
tc	966.28	K	Joback Method
tf	529.81	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.35	J/mol×K	782.91	Joback Method
cpg	729.66	J/mol×K	813.47	Joback Method
cpg	738.15	J/mol×K	844.03	Joback Method
cpg	745.87	J/mol×K	874.60	Joback Method
cpg	752.89	J/mol×K	905.16	Joback Method
cpg	759.26	J/mol×K	935.72	Joback Method
cpg	765.03	J/mol×K	966.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376237&Units=SI

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