Coniferyl alcohol, bis(pentafluoropropionate)

Inchi: InChI=1S/C16H10F10O5/c1-29-10-7-8(3-2-6-30-11(27)13(17,18)15(21,22)23)4-5-9(10)3
InchiKey: UHRCNGVEVAKRPZ-NSCUHMNNSA-N
Formula: C16H10F10O5
SMILES: COc1cc(C=CCOC(=O)C(F)(F)C(F)(F)F)ccc1OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 472.23

Physical Properties

Property code	Value	Unit	Source
gf	-2252.37	kJ/mol	Joback Method
hf	-2660.68	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	62.14	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.552		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1634.00		NIST Webbook
tb	761.06	K	Joback Method
tc	941.51	K	Joback Method
tf	498.59	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.68	J/mol×K	761.06	Joback Method
cpg	746.13	J/mol×K	791.13	Joback Method
cpg	755.77	J/mol×K	821.21	Joback Method
cpg	764.67	J/mol×K	851.28	Joback Method
cpg	772.88	J/mol×K	881.36	Joback Method
cpg	780.46	J/mol×K	911.43	Joback Method
cpg	787.48	J/mol×K	941.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375740&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