Coniferyl alcohol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C18H10F14O5/c1-35-10-7-8(3-2-6-36-11(33)13(19,20)15(23,24)17(27,28)29)4
InchiKey: SEPCGRZKBLLNAP-NSCUHMNNSA-N
Formula: C18H10F14O5
SMILES: COc1cc(C=CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F)ccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 572.25

Physical Properties

Property code	Value	Unit	Source
gf	-3009.09	kJ/mol	Joback Method
hf	-3503.90	kJ/mol	Joback Method
hfus	41.24	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	5.823		Crippen Method
mcvol	281.950	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	797.44	K	Joback Method
tc	977.69	K	Joback Method
tf	528.33	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.55	J/mol×K	797.44	Joback Method
cpg	888.73	J/mol×K	827.48	Joback Method
cpg	898.09	J/mol×K	857.52	Joback Method
cpg	906.72	J/mol×K	887.57	Joback Method
cpg	914.72	J/mol×K	917.61	Joback Method
cpg	922.17	J/mol×K	947.65	Joback Method
cpg	929.16	J/mol×K	977.69	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=U375739&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