

Propane-1,3-diyl bis(2,3,4,5,6-pentafluorobenzoate)

Inchi: InChI=1S/C17H6F10O4/c18-6-4(7(19)11(23)14(26)10(6)22)16(28)30-2-1-3-31-17(29)5-8
InchiKey: WLUOMTVGHIINLA-UHFFFAOYSA-N
Formula: C17H6F10O4
SMILES: O=C(OCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 464.21

Physical Properties

Property code	Value	Unit	Source
gf	-2195.16	kJ/mol	Joback Method
hf	-2486.55	kJ/mol	Joback Method
hfus	60.35	kJ/mol	Joback Method
hvap	74.75	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	4.482		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	1959.00		NIST Webbook
rinpol	1959.00		NIST Webbook
tb	836.80	K	Joback Method
tc	1025.90	K	Joback Method
tf	609.61	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.61	J/mol×K	836.80	Joback Method
cpg	684.85	J/mol×K	868.32	Joback Method
cpg	693.30	J/mol×K	899.83	Joback Method
cpg	700.93	J/mol×K	931.35	Joback Method
cpg	707.73	J/mol×K	962.86	Joback Method
cpg	713.69	J/mol×K	994.38	Joback Method
cpg	718.79	J/mol×K	1025.90	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=U373580&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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