1,5-Pentanediol, O,O'-bis(3-chloro-2-fluorobenzoyl)-

Inchi: InChI=1S/C19H16Cl2F2O4/c20-14-8-4-6-12(16(14)22)18(24)26-10-2-1-3-11-27-19(25)13

InchiKey: WWMLEEMKWONWSV-UHFFFAOYSA-N

Formula: C19H16Cl2F2O4

SMILES: O=C(OCCCCCOC(=O)c1cccc(Cl)c1F)c1cccc(Cl)c1F

Mol. weight [g/mol]: 417.23

Physical Properties

Property code	Value	Unit	Source
gf	-585.92	kJ/mol	Joback Method
hf	-921.61	kJ/mol	Joback Method
hfus	51.62	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.456		Crippen Method
mcvol	273.950	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	3026.00		NIST Webbook
tb	933.38	K	Joback Method
tc	1156.94	K	Joback Method
tf	612.15	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.56	J/mol×K	933.38	Joback Method
cpg	788.81	J/mol×K	970.64	Joback Method
cpg	797.89	J/mol×K	1007.90	Joback Method
cpg	805.83	J/mol×K	1045.16	Joback Method
cpg	812.64	J/mol×K	1082.42	Joback Method
cpg	818.34	J/mol×K	1119.68	Joback Method
cpg	822.96	J/mol×K	1156.94	Joback Method

Sources

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=U357336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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