Dodecyl 2,3,4,5,6-pentafluorobenzoate

Other names: dodecyl pentafluorobenzoate
Inchi: InChI=1S/C19H25F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-26-19(25)13-14(20)16(22)18(24)17
InchiKey: LOVOYRLAEIBBPN-UHFFFAOYSA-N
Formula: C19H25F5O2
SMILES: CCCCCCCCCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 380.39

Physical Properties

Property code	Value	Unit	Source
gf	-1034.61	kJ/mol	Joback Method
hf	-1481.66	kJ/mol	Joback Method
hfus	55.25	kJ/mol	Joback Method
hvap	68.55	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	6.460		Crippen Method
mcvol	271.100	ml/mol	McGowan Method
pc	1137.50	kPa	Joback Method
rinpol	2005.00		NIST Webbook
ripol	2293.00		NIST Webbook
tb	758.34	K	Joback Method
tc	933.16	K	Joback Method
tf	468.02	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.82	J/mol×K	758.34	Joback Method
cpg	820.16	J/mol×K	787.48	Joback Method
cpg	834.70	J/mol×K	816.61	Joback Method
cpg	848.46	J/mol×K	845.75	Joback Method
cpg	861.44	J/mol×K	874.89	Joback Method
cpg	873.66	J/mol×K	904.02	Joback Method
cpg	885.14	J/mol×K	933.16	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=U372790&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume