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

Inchi: InChI=1S/C10H7F5O3/c1-17-2-3-18-10(16)4-5(11)7(13)9(15)8(14)6(4)12/h2-3H2,1H3
InchiKey: QZFWGQDBNKUOLE-UHFFFAOYSA-N
Formula: C10H7F5O3
SMILES: COCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 270.15

Physical Properties

Property code	Value	Unit	Source
gf	-1215.39	kJ/mol	Joback Method
hf	-1428.12	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	50.92	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.185		Crippen Method
mcvol	150.160	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1269.00		NIST Webbook
rinpol	1269.00		NIST Webbook
tb	574.84	K	Joback Method
tc	747.12	K	Joback Method
tf	388.82	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.74	J/mol×K	574.84	Joback Method
cpg	372.19	J/mol×K	603.55	Joback Method
cpg	381.29	J/mol×K	632.27	Joback Method
cpg	390.05	J/mol×K	660.98	Joback Method
cpg	398.45	J/mol×K	689.69	Joback Method
cpg	406.47	J/mol×K	718.40	Joback Method
cpg	414.10	J/mol×K	747.12	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=U378308&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume