2,6-Difluorobenzoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C10H7ClF2O2/c11-5-2-6-15-10(14)9-7(12)3-1-4-8(9)13/h1-5H,6H2/b5-2+

InchiKey: WKAFCDBHJQUKJC-GORDUTHDSA-N

Formula: C10H7ClF2O2

SMILES: O=C(OCC=CCl)c1c(F)cccc1F

Mol. weight [g/mol]: 232.61

Physical Properties

Property code	Value	Unit	Source
gf	-428.78	kJ/mol	Joback Method
hf	-571.68	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	53.32	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.874		Crippen Method
mcvol	146.920	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1491.60		NIST Webbook
rinpol	1491.60		NIST Webbook
tb	581.26	K	Joback Method
tc	788.87	K	Joback Method
tf	352.10	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.57	J/mol×K	581.26	Joback Method
cpg	331.97	J/mol×K	615.86	Joback Method
cpg	341.74	J/mol×K	650.46	Joback Method
cpg	350.91	J/mol×K	685.06	Joback Method
cpg	359.48	J/mol×K	719.66	Joback Method
cpg	367.49	J/mol×K	754.26	Joback Method
cpg	374.95	J/mol×K	788.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292590&Units=SI
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

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