Fumaric acid, 2,5-dichlorophenyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H9Cl2F3O4/c1-7(13(16,17)18)21-11(19)4-5-12(20)22-10-6-8(14)2-3-9(10)1

InchiKey: CHHUAKAMGRSGHY-SNAWJCMRSA-N

Formula: C13H9Cl2F3O4

SMILES: CC(OC(=O)C=CC(=O)Oc1cc(Cl)ccc1Cl)C(F)(F)F

Mol. weight [g/mol]: 357.11

Physical Properties

Property code	Value	Unit	Source
gf	-843.78	kJ/mol	Joback Method
hf	-1104.28	kJ/mol	Joback Method
hfus	35.16	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.949		Crippen Method
mcvol	210.640	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	759.22	K	Joback Method
tc	971.58	K	Joback Method
tf	476.00	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.74	J/mol×K	759.22	Joback Method
cpg	546.69	J/mol×K	794.61	Joback Method
cpg	555.82	J/mol×K	830.01	Joback Method
cpg	564.19	J/mol×K	865.40	Joback Method
cpg	571.82	J/mol×K	900.80	Joback Method
cpg	578.75	J/mol×K	936.19	Joback Method
cpg	585.03	J/mol×K	971.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405961&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