Fumaric acid, 2,4,6-trichlorophenyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H8Cl3F3O4/c1-6(13(17,18)19)22-10(20)2-3-11(21)23-12-8(15)4-7(14)5-9(1

InchiKey: QICJDILZYKHBSN-NSCUHMNNSA-N

Formula: C13H8Cl3F3O4

SMILES: CC(OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)C(F)(F)F

Mol. weight [g/mol]: 391.55

Physical Properties

Property code	Value	Unit	Source
gf	-865.34	kJ/mol	Joback Method
hf	-1131.49	kJ/mol	Joback Method
hfus	38.97	kJ/mol	Joback Method
hvap	76.08	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.602		Crippen Method
mcvol	222.880	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	801.63	K	Joback Method
tc	1018.08	K	Joback Method
tf	518.44	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.29	J/mol×K	801.63	Joback Method
cpg	564.13	J/mol×K	837.70	Joback Method
cpg	572.20	J/mol×K	873.78	Joback Method
cpg	579.53	J/mol×K	909.85	Joback Method
cpg	586.16	J/mol×K	945.93	Joback Method
cpg	592.12	J/mol×K	982.00	Joback Method
cpg	597.44	J/mol×K	1018.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405945&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

Latest version available from:
https://www.chemeo.com/cid/116-979-7/Fumaric-acid-2-4-6-trichlorophenyl-1-1-1-trifluoroprop-2-yl-ester.pdf
Generated by Cheméo on 2024-05-16 15:55:14.786924404 +0000 UTC m=+18164163.707501716.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.