Fumaric acid, 2,6-dichlorophenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H8Cl2F4O4/c14-7-2-1-3-8(15)11(7)23-10(21)5-4-9(20)22-6-13(18,19)12(16

InchiKey: XRNWDXJNFWHLLB-SNAWJCMRSA-N

Formula: C13H8Cl2F4O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cccc1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 375.10

Physical Properties

Property code	Value	Unit	Source
gf	-1038.59	kJ/mol	Joback Method
hf	-1300.39	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.899		Crippen Method
mcvol	212.410	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tb	758.49	K	Joback Method
tc	963.59	K	Joback Method
tf	476.59	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.56	J/mol×K	758.49	Joback Method
cpg	554.08	J/mol×K	792.67	Joback Method
cpg	562.83	J/mol×K	826.86	Joback Method
cpg	570.85	J/mol×K	861.04	Joback Method
cpg	578.18	J/mol×K	895.22	Joback Method
cpg	584.84	J/mol×K	929.40	Joback Method
cpg	590.89	J/mol×K	963.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405859&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

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