Glutaric acid, 2,2,3,3-tetrafluoropropyl 2,5-dichlorophenyl ester

Inchi: InChI=1S/C14H12Cl2F4O4/c15-8-4-5-9(16)10(6-8)24-12(22)3-1-2-11(21)23-7-14(19,20)1

InchiKey: CAAKKJGTCCDSNQ-UHFFFAOYSA-N

Formula: C14H12Cl2F4O4

SMILES: O=C(CCCC(=O)Oc1cc(Cl)ccc1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 391.14

Physical Properties

Property code	Value	Unit	Source
gf	-1110.39	kJ/mol	Joback Method
hf	-1438.25	kJ/mol	Joback Method
hfus	40.63	kJ/mol	Joback Method
hvap	72.49	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.513		Crippen Method
mcvol	230.800	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook
tb	777.21	K	Joback Method
tc	975.36	K	Joback Method
tf	492.94	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.52	J/mol×K	777.21	Joback Method
cpg	633.12	J/mol×K	810.24	Joback Method
cpg	642.90	J/mol×K	843.26	Joback Method
cpg	651.88	J/mol×K	876.29	Joback Method
cpg	660.09	J/mol×K	909.31	Joback Method
cpg	667.55	J/mol×K	942.34	Joback Method
cpg	674.29	J/mol×K	975.36	Joback Method

Sources

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=U392050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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