Glutaric acid, 2,2-dichloroethyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C14H15Cl2FO5/c1-20-11-7-9(17)5-6-10(11)22-14(19)4-2-3-13(18)21-8-12(15)16

InchiKey: IYSWFQPTSOFWRR-UHFFFAOYSA-N

Formula: C14H15Cl2FO5

SMILES: COc1cc(F)ccc1OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 353.17

Physical Properties

Property code	Value	Unit	Source
gf	-633.80	kJ/mol	Joback Method
hf	-973.39	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.257		Crippen Method
mcvol	231.360	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
tb	805.05	K	Joback Method
tc	1013.68	K	Joback Method
tf	510.98	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.88	J/mol×K	805.05	Joback Method
cpg	634.34	J/mol×K	839.82	Joback Method
cpg	644.85	J/mol×K	874.59	Joback Method
cpg	654.40	J/mol×K	909.36	Joback Method
cpg	662.97	J/mol×K	944.14	Joback Method
cpg	670.56	J/mol×K	978.91	Joback Method
cpg	677.16	J/mol×K	1013.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393442&Units=SI

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