Glutaric acid, 3-chlorophenyl 2-fluoroethyl ester

Inchi: InChI=1S/C13H14ClFO4/c14-10-3-1-4-11(9-10)19-13(17)6-2-5-12(16)18-8-7-15/h1,3-4,9

InchiKey: YQMPZFVLQIDNCC-UHFFFAOYSA-N

Formula: C13H14ClFO4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCCF

Mol. weight [g/mol]: 288.70

Physical Properties

Property code	Value	Unit	Source
gf	-513.22	kJ/mol	Joback Method
hf	-788.04	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.928		Crippen Method
mcvol	199.160	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tb	717.78	K	Joback Method
tc	921.86	K	Joback Method
tf	450.04	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.97	J/mol×K	717.78	Joback Method
cpg	533.29	J/mol×K	751.79	Joback Method
cpg	544.79	J/mol×K	785.81	Joback Method
cpg	555.48	J/mol×K	819.82	Joback Method
cpg	565.36	J/mol×K	853.83	Joback Method
cpg	574.45	J/mol×K	887.84	Joback Method
cpg	582.74	J/mol×K	921.86	Joback Method

Sources

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=U393715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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