Glutaric acid, 2-fluorophenyl 2-fluoroethyl ester

Inchi: InChI=1S/C13H14F2O4/c14-8-9-18-12(16)6-3-7-13(17)19-11-5-2-1-4-10(11)15/h1-2,4-5H

InchiKey: OHLNBLHDDOVMST-UHFFFAOYSA-N

Formula: C13H14F2O4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCCF

Mol. weight [g/mol]: 272.24

Physical Properties

Property code	Value	Unit	Source
gf	-696.10	kJ/mol	Joback Method
hf	-968.41	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.414		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
tb	679.62	K	Joback Method
tc	872.58	K	Joback Method
tf	420.71	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.53	J/mol×K	679.62	Joback Method
cpg	516.27	J/mol×K	711.78	Joback Method
cpg	528.25	J/mol×K	743.94	Joback Method
cpg	539.50	J/mol×K	776.10	Joback Method
cpg	550.00	J/mol×K	808.26	Joback Method
cpg	559.77	J/mol×K	840.42	Joback Method
cpg	568.82	J/mol×K	872.58	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=U393711&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