Glutaric acid, 2-ethylhexyl 2-fluoroethyl ester

Inchi: InChI=1S/C15H27FO4/c1-3-5-7-13(4-2)12-20-15(18)9-6-8-14(17)19-11-10-16/h13H,3-12
InchiKey: VLMRTSFIKYZUFT-UHFFFAOYSA-N
Formula: C15H27FO4
SMILES: CCCCC(CC)COC(=O)CCCC(=O)OCCF
Mol. weight [g/mol]: 290.37

Physical Properties

Property code	Value	Unit	Source
gf	-589.67	kJ/mol	Joback Method
hf	-1043.92	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.429		Crippen Method
mcvol	238.860	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	1819.00		NIST Webbook
rinpol	1819.00		NIST Webbook
tb	694.01	K	Joback Method
tc	867.11	K	Joback Method
tf	388.72	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.59	J/mol×K	694.01	Joback Method
cpg	701.42	J/mol×K	722.86	Joback Method
cpg	716.50	J/mol×K	751.71	Joback Method
cpg	730.82	J/mol×K	780.56	Joback Method
cpg	744.40	J/mol×K	809.41	Joback Method
cpg	757.24	J/mol×K	838.26	Joback Method
cpg	769.35	J/mol×K	867.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393712&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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