Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-ethylcyclohexyl ester

Inchi: InChI=1S/C16H24F4O4/c1-2-11-6-3-4-7-12(11)24-14(22)9-5-8-13(21)23-10-16(19,20)15

InchiKey: UXPYQKPUUIGQOB-UHFFFAOYSA-N

Formula: C16H24F4O4

SMILES: CCC1CCCCC1OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 356.35

Physical Properties

Property code	Value	Unit	Source
gf	-1146.10	kJ/mol	Joback Method
hf	-1627.66	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.112		Crippen Method
mcvol	247.400	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
tb	726.35	K	Joback Method
tc	908.76	K	Joback Method
tf	407.32	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.65	J/mol×K	726.35	Joback Method
cpg	781.65	J/mol×K	756.75	Joback Method
cpg	797.61	J/mol×K	787.15	Joback Method
cpg	812.55	J/mol×K	817.55	Joback Method
cpg	826.48	J/mol×K	847.96	Joback Method
cpg	839.43	J/mol×K	878.36	Joback Method
cpg	851.42	J/mol×K	908.76	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=U405476&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