Glutaric acid, 2-ethylcyclohexyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C16H25F3O4/c1-3-12-7-4-5-8-13(12)23-15(21)10-6-9-14(20)22-11(2)16(17,18
InchiKey: QSWNEEACYTWENE-UHFFFAOYSA-N
Formula: C16H25F3O4
SMILES: CCC1CCCCC1OC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 338.36

Physical Properties

Property code	Value	Unit	Source
gf	-951.29	kJ/mol	Joback Method
hf	-1431.55	kJ/mol	Joback Method
hfus	33.98	kJ/mol	Joback Method
hvap	65.51	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.163		Crippen Method
mcvol	245.630	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
tb	727.08	K	Joback Method
tc	914.78	K	Joback Method
tf	406.73	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.93	J/mol×K	727.08	Joback Method
cpg	774.49	J/mol×K	758.36	Joback Method
cpg	790.95	J/mol×K	789.65	Joback Method
cpg	806.33	J/mol×K	820.93	Joback Method
cpg	820.66	J/mol×K	852.21	Joback Method
cpg	833.96	J/mol×K	883.50	Joback Method
cpg	846.25	J/mol×K	914.78	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=U405475&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