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

Inchi: InChI=1S/C16H18F4O4/c1-2-11-6-3-4-7-12(11)24-14(22)9-5-8-13(21)23-10-16(19,20)15

InchiKey: FOWAYKULBBLJDV-UHFFFAOYSA-N

Formula: C16H18F4O4

SMILES: CCc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1060.06	kJ/mol	Joback Method
hf	-1436.58	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	67.51	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.768		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook
tb	743.13	K	Joback Method
tc	930.69	K	Joback Method
tf	443.12	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.14	J/mol×K	743.13	Joback Method
cpg	695.65	J/mol×K	774.39	Joback Method
cpg	708.27	J/mol×K	805.65	Joback Method
cpg	720.04	J/mol×K	836.91	Joback Method
cpg	730.97	J/mol×K	868.17	Joback Method
cpg	741.10	J/mol×K	899.43	Joback Method
cpg	750.45	J/mol×K	930.69	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=U390840&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