Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C15H12F8O4/c16-12-8(15(21,22)23)3-1-4-9(12)27-11(25)6-2-5-10(24)26-7-14

InchiKey: KLCKTNCFVKFKOC-UHFFFAOYSA-N

Formula: C15H12F8O4

SMILES: O=C(CCCC(=O)Oc1cccc(C(F)(F)F)c1F)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 408.24

Physical Properties

Property code	Value	Unit	Source
gf	-1854.51	kJ/mol	Joback Method
hf	-2220.60	kJ/mol	Joback Method
hfus	39.73	kJ/mol	Joback Method
hvap	61.38	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.364		Crippen Method
mcvol	227.490	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	719.08	K	Joback Method
tc	893.89	K	Joback Method
tf	449.15	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.94	J/mol×K	719.08	Joback Method
cpg	672.49	J/mol×K	748.21	Joback Method
cpg	683.29	J/mol×K	777.35	Joback Method
cpg	693.34	J/mol×K	806.48	Joback Method
cpg	702.69	J/mol×K	835.62	Joback Method
cpg	711.37	J/mol×K	864.75	Joback Method
cpg	719.40	J/mol×K	893.89	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=U393612&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