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

Inchi: InChI=1S/C16H16F4O5/c1-10(21)11-5-2-3-6-12(11)25-14(23)8-4-7-13(22)24-9-16(19,20
InchiKey: LMZYJNCXYXRQDJ-UHFFFAOYSA-N
Formula: C16H16F4O5
SMILES: CC(=O)c1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 364.29

Physical Properties

Property code	Value	Unit	Source
gf	-1188.98	kJ/mol	Joback Method
hf	-1549.16	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.409		Crippen Method
mcvol	236.070	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	2073.00		NIST Webbook
rinpol	2073.00		NIST Webbook
tb	797.00	K	Joback Method
tc	992.18	K	Joback Method
tf	493.05	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.21	J/mol×K	797.00	Joback Method
cpg	709.18	J/mol×K	829.53	Joback Method
cpg	720.23	J/mol×K	862.06	Joback Method
cpg	730.39	J/mol×K	894.59	Joback Method
cpg	739.69	J/mol×K	927.12	Joback Method
cpg	748.17	J/mol×K	959.65	Joback Method
cpg	755.84	J/mol×K	992.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392042&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