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

Inchi: InChI=1S/C16H18F4O4/c17-15(18)16(19,20)11-24-14(22)8-4-7-13(21)23-10-9-12-5-2-1-

InchiKey: IVLGMOSBMZPFFR-UHFFFAOYSA-N

Formula: C16H18F4O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCCc1ccccc1

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1050.43	kJ/mol	Joback Method
hf	-1425.11	kJ/mol	Joback Method
hfus	38.19	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.386		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	1906.00		NIST Webbook
rinpol	1906.00		NIST Webbook
tb	738.15	K	Joback Method
tc	924.86	K	Joback Method
tf	430.60	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.00	J/mol×K	738.15	Joback Method
cpg	696.62	J/mol×K	769.27	Joback Method
cpg	709.34	J/mol×K	800.39	Joback Method
cpg	721.19	J/mol×K	831.51	Joback Method
cpg	732.20	J/mol×K	862.62	Joback Method
cpg	742.41	J/mol×K	893.74	Joback Method
cpg	751.83	J/mol×K	924.86	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=U391784&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