Glutaric acid, 2,2,3,3-tetrafluoropropyl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C16H18F4O5/c1-10-6-7-11(23-2)12(8-10)25-14(22)5-3-4-13(21)24-9-16(19,20)

InchiKey: DWQXKXAHCJXCHK-UHFFFAOYSA-N

Formula: C16H18F4O5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 366.30

Physical Properties

Property code	Value	Unit	Source
gf	-1174.69	kJ/mol	Joback Method
hf	-1580.27	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.523		Crippen Method
mcvol	240.370	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	770.53	K	Joback Method
tc	959.51	K	Joback Method
tf	477.87	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.55	J/mol×K	770.53	Joback Method
cpg	721.67	J/mol×K	802.03	Joback Method
cpg	733.89	J/mol×K	833.52	Joback Method
cpg	745.22	J/mol×K	865.02	Joback Method
cpg	755.68	J/mol×K	896.52	Joback Method
cpg	765.27	J/mol×K	928.01	Joback Method
cpg	774.00	J/mol×K	959.51	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=U393919&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