Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-methoxybenzyl ester

Inchi: InChI=1S/C16H18F4O5/c1-23-12-7-5-11(6-8-12)9-24-13(21)3-2-4-14(22)25-10-16(19,20)15(17)18/h5-8,15H,2-4,9-10H2,1H3

InchiKey: MRKNHBAJYXSXFS-UHFFFAOYSA-N

Formula: C16H18F4O5

SMILES: COc1ccc(COC(=O)CCCC(=O)OCC(F)(F)C(F)F)cc1

Mol. weight [g/mol]: 366.30

Physical Properties

Property code	Value	Unit	Source
gf	-1165.06	kJ/mol	Joback Method
hf	-1568.80	kJ/mol	Joback Method
hfus	38.99	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.352		Crippen Method
mcvol	240.370	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook
tb	765.55	K	Joback Method
tc	953.67	K	Joback Method
tf	465.35	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.51	J/mol×K	765.55	Joback Method
cpg	722.72	J/mol×K	796.90	Joback Method
cpg	735.03	J/mol×K	828.26	Joback Method
cpg	746.45	J/mol×K	859.61	Joback Method
cpg	756.99	J/mol×K	890.96	Joback Method
cpg	766.66	J/mol×K	922.32	Joback Method
cpg	775.50	J/mol×K	953.67	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=U391737&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