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

Inchi: InChI=1S/C15H16F4O5/c1-22-10-5-2-3-6-11(10)24-13(21)8-4-7-12(20)23-9-15(18,19)14

InchiKey: PADZLJNIAWVDFP-UHFFFAOYSA-N

Formula: C15H16F4O5

SMILES: COc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 352.28

Physical Properties

Property code	Value	Unit	Source
gf	-1173.48	kJ/mol	Joback Method
hf	-1548.16	kJ/mol	Joback Method
hfus	36.40	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.215		Crippen Method
mcvol	226.280	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1938.00		NIST Webbook
rinpol	1938.00		NIST Webbook
tb	742.67	K	Joback Method
tc	930.78	K	Joback Method
tf	454.08	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.76	J/mol×K	742.67	Joback Method
cpg	667.62	J/mol×K	774.02	Joback Method
cpg	679.61	J/mol×K	805.37	Joback Method
cpg	690.74	J/mol×K	836.73	Joback Method
cpg	701.03	J/mol×K	868.08	Joback Method
cpg	710.49	J/mol×K	899.43	Joback Method
cpg	719.15	J/mol×K	930.78	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=U391751&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