Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C15H15BrF4O5/c1-23-11-7-9(16)5-6-10(11)25-13(22)4-2-3-12(21)24-8-15(19,

InchiKey: CCASVMMTWWIZPZ-UHFFFAOYSA-N

Formula: C15H15BrF4O5

SMILES: COc1cc(Br)ccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 431.17

Physical Properties

Property code	Value	Unit	Source
gf	-1168.79	kJ/mol	Joback Method
hf	-1533.30	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	74.79	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.977		Crippen Method
mcvol	243.780	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
tb	813.81	K	Joback Method
tc	1013.64	K	Joback Method
tf	526.40	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.91	J/mol×K	813.81	Joback Method
cpg	701.15	J/mol×K	847.12	Joback Method
cpg	711.49	J/mol×K	880.42	Joback Method
cpg	720.95	J/mol×K	913.73	Joback Method
cpg	729.54	J/mol×K	947.03	Joback Method
cpg	737.29	J/mol×K	980.34	Joback Method
cpg	744.22	J/mol×K	1013.64	Joback Method

Sources

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=U393587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume