Glutaric acid, 1,1,1-trifluoroprop-2-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C15H16BrF3O5/c1-9(15(17,18)19)23-13(20)4-3-5-14(21)24-11-7-6-10(16)8-12

InchiKey: OMZGKTDDYSUQFL-UHFFFAOYSA-N

Formula: C15H16BrF3O5

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

Mol. weight [g/mol]: 413.18

Physical Properties

Property code	Value	Unit	Source
gf	-973.98	kJ/mol	Joback Method
hf	-1337.19	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	75.61	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.027		Crippen Method
mcvol	242.010	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	814.54	K	Joback Method
tc	1019.64	K	Joback Method
tf	525.81	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.34	J/mol×K	814.54	Joback Method
cpg	693.97	J/mol×K	848.72	Joback Method
cpg	704.66	J/mol×K	882.91	Joback Method
cpg	714.43	J/mol×K	917.09	Joback Method
cpg	723.30	J/mol×K	951.27	Joback Method
cpg	731.28	J/mol×K	985.46	Joback Method
cpg	738.40	J/mol×K	1019.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393585&Units=SI
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

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