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

Inchi: InChI=1S/C14H12BrF5O4/c15-9-6-8(16)4-5-10(9)24-12(22)3-1-2-11(21)23-7-14(19,20)13

InchiKey: UUAOWEDIQQMMBO-UHFFFAOYSA-N

Formula: C14H12BrF5O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)cc1Br)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 419.14

Physical Properties

Property code	Value	Unit	Source
gf	-1267.02	kJ/mol	Joback Method
hf	-1576.55	kJ/mol	Joback Method
hfus	40.60	kJ/mol	Joback Method
hvap	69.34	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.107		Crippen Method
mcvol	225.590	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook
tb	767.78	K	Joback Method
tc	962.38	K	Joback Method
tf	493.49	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.91	J/mol×K	767.78	Joback Method
cpg	628.65	J/mol×K	800.21	Joback Method
cpg	638.60	J/mol×K	832.65	Joback Method
cpg	647.79	J/mol×K	865.08	Joback Method
cpg	656.25	J/mol×K	897.52	Joback Method
cpg	664.00	J/mol×K	929.95	Joback Method
cpg	671.07	J/mol×K	962.38	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=U391822&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume