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

Inchi: InChI=1S/C14H13BrF4O4/c15-9-4-6-10(7-5-9)23-12(21)3-1-2-11(20)22-8-14(18,19)13(16

InchiKey: DRCQEMBXHVKVRJ-UHFFFAOYSA-N

Formula: C14H13BrF4O4

SMILES: O=C(CCCC(=O)Oc1ccc(Br)cc1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 401.15

Physical Properties

Property code	Value	Unit	Source
gf	-1062.58	kJ/mol	Joback Method
hf	-1368.97	kJ/mol	Joback Method
hfus	37.91	kJ/mol	Joback Method
hvap	69.49	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.968		Crippen Method
mcvol	223.820	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	763.53	K	Joback Method
tc	963.14	K	Joback Method
tf	480.38	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.54	J/mol×K	763.53	Joback Method
cpg	622.78	J/mol×K	796.80	Joback Method
cpg	633.19	J/mol×K	830.07	Joback Method
cpg	642.78	J/mol×K	863.34	Joback Method
cpg	651.60	J/mol×K	896.60	Joback Method
cpg	659.68	J/mol×K	929.87	Joback Method
cpg	667.05	J/mol×K	963.14	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=U393283&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