Glutaric acid, cyclohexylmethyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C18H22BrFO4/c19-15-11-14(20)9-10-16(15)24-18(22)8-4-7-17(21)23-12-13-5-
InchiKey: YTUFOOLPRFGFFZ-UHFFFAOYSA-N
Formula: C18H22BrFO4
SMILES: O=C(CCCC(=O)Oc1ccc(F)cc1Br)OCC1CCCCC1
Mol. weight [g/mol]: 401.27

Physical Properties

Property code	Value	Unit	Source
gf	-430.05	kJ/mol	Joback Method
hf	-806.32	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	83.62	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.787		Crippen Method
mcvol	264.010	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	885.44	K	Joback Method
tc	1111.94	K	Joback Method
tf	556.17	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.03	J/mol×K	885.44	Joback Method
cpg	815.13	J/mol×K	923.19	Joback Method
cpg	827.86	J/mol×K	960.94	Joback Method
cpg	839.24	J/mol×K	998.69	Joback Method
cpg	849.31	J/mol×K	1036.44	Joback Method
cpg	858.09	J/mol×K	1074.19	Joback Method
cpg	865.63	J/mol×K	1111.94	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=U391833&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