Glutaric acid, naphth-2-ylmethyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C22H18BrFO4/c23-19-13-18(24)10-11-20(19)28-22(26)7-3-6-21(25)27-14-15-8

InchiKey: VREBDOONCRGWGH-UHFFFAOYSA-N

Formula: C22H18BrFO4

SMILES: O=C(CCCC(=O)Oc1ccc(F)cc1Br)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 445.28

Physical Properties

Property code	Value	Unit	Source
gf	-211.39	kJ/mol	Joback Method
hf	-527.07	kJ/mol	Joback Method
hfus	50.61	kJ/mol	Joback Method
hvap	96.67	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	5.561		Crippen Method
mcvol	288.010	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	3291.00		NIST Webbook
tb	1008.05	K	Joback Method
tc	1251.05	K	Joback Method
tf	665.51	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.81	J/mol×K	1008.05	Joback Method
cpg	861.50	J/mol×K	1048.55	Joback Method
cpg	871.19	J/mol×K	1089.05	Joback Method
cpg	879.96	J/mol×K	1129.55	Joback Method
cpg	887.89	J/mol×K	1170.05	Joback Method
cpg	895.08	J/mol×K	1210.55	Joback Method
cpg	901.61	J/mol×K	1251.05	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391842&Units=SI

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