Glutaric acid, dodec-2-en-1-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C23H32BrFO4/c1-2-3-4-5-6-7-8-9-10-11-17-28-22(26)13-12-14-23(27)29-21-1

InchiKey: RTODNQSMRWAMHN-ZHACJKMWSA-N

Formula: C23H32BrFO4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 471.40

Physical Properties

Property code	Value	Unit	Source
gf	-332.18	kJ/mol	Joback Method
hf	-846.62	kJ/mol	Joback Method
hfus	62.73	kJ/mol	Joback Method
hvap	94.28	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.904		Crippen Method
mcvol	341.020	ml/mol	McGowan Method
pc	1143.66	kPa	Joback Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tb	984.45	K	Joback Method
tc	1205.54	K	Joback Method
tf	600.06	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.62	J/mol×K	984.45	Joback Method
cpg	1090.19	J/mol×K	1021.30	Joback Method
cpg	1103.59	J/mol×K	1058.15	Joback Method
cpg	1115.88	J/mol×K	1095.00	Joback Method
cpg	1127.12	J/mol×K	1131.85	Joback Method
cpg	1137.36	J/mol×K	1168.70	Joback Method
cpg	1146.67	J/mol×K	1205.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391840&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