Glutaric acid, hept-2-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C18H24BrFO4/c1-3-4-5-7-13(2)23-17(21)8-6-9-18(22)24-16-11-10-14(20)12-15

InchiKey: FUHVWNGEWUUOOY-UHFFFAOYSA-N

Formula: C18H24BrFO4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 403.28

Physical Properties

Property code	Value	Unit	Source
gf	-456.94	kJ/mol	Joback Method
hf	-865.92	kJ/mol	Joback Method
hfus	46.05	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.176		Crippen Method
mcvol	274.870	ml/mol	McGowan Method
pc	1573.45	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	865.45	K	Joback Method
tc	1073.80	K	Joback Method
tf	533.79	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.10	J/mol×K	865.45	Joback Method
cpg	821.73	J/mol×K	900.18	Joback Method
cpg	834.30	J/mol×K	934.90	Joback Method
cpg	845.83	J/mol×K	969.63	Joback Method
cpg	856.34	J/mol×K	1004.35	Joback Method
cpg	865.86	J/mol×K	1039.08	Joback Method
cpg	874.40	J/mol×K	1073.80	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=U389774&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