Glutaric acid, 8-chlorooctyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C19H25BrClFO4/c20-16-14-15(22)10-11-17(16)26-19(24)9-7-8-18(23)25-13-6-
InchiKey: NRDLMJORAYMFRM-UHFFFAOYSA-N
Formula: C19H25BrClFO4
SMILES: O=C(CCCC(=O)Oc1ccc(F)cc1Br)OCCCCCCCCCCl
Mol. weight [g/mol]: 451.75

Physical Properties

Property code	Value	Unit	Source
gf	-458.01	kJ/mol	Joback Method
hf	-897.02	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	89.80	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	5.786		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	2924.00		NIST Webbook
tb	926.20	K	Joback Method
tc	1139.40	K	Joback Method
tf	589.98	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.28	J/mol×K	926.20	Joback Method
cpg	901.96	J/mol×K	961.73	Joback Method
cpg	913.55	J/mol×K	997.27	Joback Method
cpg	924.08	J/mol×K	1032.80	Joback Method
cpg	933.57	J/mol×K	1068.33	Joback Method
cpg	942.05	J/mol×K	1103.86	Joback Method
cpg	949.56	J/mol×K	1139.40	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=U391838&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