Glutaric acid, di(2-bromo-5-fluorobenzyl) ester

Inchi: InChI=1S/C19H16Br2F2O4/c20-16-6-4-14(22)8-12(16)10-26-18(24)2-1-3-19(25)27-11-13
InchiKey: ZUEAJRNYXZLAQV-UHFFFAOYSA-N
Formula: C19H16Br2F2O4
SMILES: O=C(CCCC(=O)OCc1cc(F)ccc1Br)OCc1cc(F)ccc1Br
Mol. weight [g/mol]: 506.13

Physical Properties

Property code	Value	Unit	Source
gf	-533.42	kJ/mol	Joback Method
hf	-837.47	kJ/mol	Joback Method
hfus	53.80	kJ/mol	Joback Method
hvap	94.64	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	5.447		Crippen Method
mcvol	284.470	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	3001.00		NIST Webbook
tb	990.84	K	Joback Method
tc	1226.50	K	Joback Method
tf	671.91	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.40	J/mol×K	990.84	Joback Method
cpg	804.69	J/mol×K	1030.12	Joback Method
cpg	812.89	J/mol×K	1069.39	Joback Method
cpg	820.03	J/mol×K	1108.67	Joback Method
cpg	826.16	J/mol×K	1147.95	Joback Method
cpg	831.32	J/mol×K	1187.23	Joback Method
cpg	835.56	J/mol×K	1226.50	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=U376866&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