Glutaric acid, 2,6-difluoro-4-bromobenzyl isobutyl ester

Inchi: InChI=1S/C16H19BrF2O4/c1-10(2)8-22-15(20)4-3-5-16(21)23-9-12-13(18)6-11(17)7-14(
InchiKey: FBWSLBSCKKSTTF-UHFFFAOYSA-N
Formula: C16H19BrF2O4
SMILES: CC(C)COC(=O)CCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 393.22

Physical Properties

Property code	Value	Unit	Source
gf	-678.22	kJ/mol	Joback Method
hf	-1032.22	kJ/mol	Joback Method
hfus	43.57	kJ/mol	Joback Method
hvap	78.20	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.140		Crippen Method
mcvol	248.460	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	823.94	K	Joback Method
tc	1028.31	K	Joback Method
tf	524.36	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.87	J/mol×K	823.94	Joback Method
cpg	713.45	J/mol×K	858.00	Joback Method
cpg	725.09	J/mol×K	892.06	Joback Method
cpg	735.81	J/mol×K	926.13	Joback Method
cpg	745.61	J/mol×K	960.19	Joback Method
cpg	754.51	J/mol×K	994.25	Joback Method
cpg	762.52	J/mol×K	1028.31	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=U376818&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