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

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

Physical Properties

Property code	Value	Unit	Source
gf	-675.78	kJ/mol	Joback Method
hf	-1026.94	kJ/mol	Joback Method
hfus	47.09	kJ/mol	Joback Method
hvap	78.58	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.284		Crippen Method
mcvol	248.460	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	824.38	K	Joback Method
tc	1026.60	K	Joback Method
tf	539.36	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.30	J/mol×K	824.38	Joback Method
cpg	712.75	J/mol×K	858.08	Joback Method
cpg	724.30	J/mol×K	891.79	Joback Method
cpg	734.96	J/mol×K	925.49	Joback Method
cpg	744.73	J/mol×K	959.19	Joback Method
cpg	753.62	J/mol×K	992.89	Joback Method
cpg	761.66	J/mol×K	1026.60	Joback Method

Sources

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=U376819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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