Glutaric acid, di(2,6-difluoro-4-bromobenzyl) ester

Inchi: InChI=1S/C19H14Br2F4O4/c20-10-4-14(22)12(15(23)5-10)8-28-18(26)2-1-3-19(27)29-9-
InchiKey: PFRUTQCAWKNKEX-UHFFFAOYSA-N
Formula: C19H14Br2F4O4
SMILES: O=C(CCCC(=O)OCc1c(F)cc(Br)cc1F)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 542.11

Physical Properties

Property code	Value	Unit	Source
gf	-942.30	kJ/mol	Joback Method
hf	-1252.63	kJ/mol	Joback Method
hfus	59.18	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	5.725		Crippen Method
mcvol	288.010	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	2918.00		NIST Webbook
tb	999.34	K	Joback Method
tc	1228.93	K	Joback Method
tf	698.13	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.57	J/mol×K	999.34	Joback Method
cpg	814.05	J/mol×K	1037.60	Joback Method
cpg	821.44	J/mol×K	1075.87	Joback Method
cpg	827.77	J/mol×K	1114.13	Joback Method
cpg	833.06	J/mol×K	1152.40	Joback Method
cpg	837.34	J/mol×K	1190.66	Joback Method
cpg	840.65	J/mol×K	1228.93	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=U376833&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