Glutaric acid, 2,6-difluoro-4-bromobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H25BrF2O4/c1-4-6-17(12(2)3)26-19(24)8-5-7-18(23)25-11-14-15(21)9-13(

InchiKey: FAETYQWUDZLMPJ-UHFFFAOYSA-N

Formula: C19H25BrF2O4

SMILES: CCCC(OC(=O)CCCC(=O)OCc1c(F)cc(Br)cc1F)C(C)C

Mol. weight [g/mol]: 435.30

Physical Properties

Property code	Value	Unit	Source
gf	-655.40	kJ/mol	Joback Method
hf	-1099.42	kJ/mol	Joback Method
hfus	47.81	kJ/mol	Joback Method
hvap	84.49	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.309		Crippen Method
mcvol	290.730	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2435.00		NIST Webbook
rinpol	2435.00		NIST Webbook
tb	892.14	K	Joback Method
tc	1099.86	K	Joback Method
tf	543.17	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.80	J/mol×K	892.14	Joback Method
cpg	886.30	J/mol×K	926.76	Joback Method
cpg	898.70	J/mol×K	961.38	Joback Method
cpg	910.00	J/mol×K	996.00	Joback Method
cpg	920.24	J/mol×K	1030.62	Joback Method
cpg	929.43	J/mol×K	1065.24	Joback Method
cpg	937.59	J/mol×K	1099.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376821&Units=SI
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

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