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

Inchi: InChI=1S/C17H21BrF2O4/c1-2-3-4-8-23-16(21)6-5-7-17(22)24-11-13-14(19)9-12(18)10-

InchiKey: UUYIOATUHYYMFM-UHFFFAOYSA-N

Formula: C17H21BrF2O4

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

Mol. weight [g/mol]: 407.25

Physical Properties

Property code	Value	Unit	Source
gf	-667.36	kJ/mol	Joback Method
hf	-1047.58	kJ/mol	Joback Method
hfus	49.68	kJ/mol	Joback Method
hvap	80.81	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.674		Crippen Method
mcvol	262.550	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2380.00		NIST Webbook
tb	847.26	K	Joback Method
tc	1049.75	K	Joback Method
tf	550.63	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.62	J/mol×K	847.26	Joback Method
cpg	769.41	J/mol×K	881.01	Joback Method
cpg	781.24	J/mol×K	914.76	Joback Method
cpg	792.14	J/mol×K	948.51	Joback Method
cpg	802.10	J/mol×K	982.26	Joback Method
cpg	811.16	J/mol×K	1016.00	Joback Method
cpg	819.32	J/mol×K	1049.75	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=U376820&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