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

Inchi: InChI=1S/C27H41BrF2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-33-26(31)16-15-17-27(

InchiKey: ZDYMHRIRADVLGP-UHFFFAOYSA-N

Formula: C27H41BrF2O4

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

Mol. weight [g/mol]: 547.51

Physical Properties

Property code	Value	Unit	Source
gf	-583.16	kJ/mol	Joback Method
hf	-1253.98	kJ/mol	Joback Method
hfus	75.58	kJ/mol	Joback Method
hvap	103.07	kJ/mol	Joback Method
log10ws	-10.27		Crippen Method
logp	8.575		Crippen Method
mcvol	403.450	ml/mol	McGowan Method
pc	838.70	kPa	Joback Method
rinpol	3417.00		NIST Webbook
tb	1076.06	K	Joback Method
tc	1330.74	K	Joback Method
tf	663.33	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1356.60	J/mol×K	1076.06	Joback Method
cpg	1372.65	J/mol×K	1118.51	Joback Method
cpg	1386.82	J/mol×K	1160.95	Joback Method
cpg	1399.19	J/mol×K	1203.40	Joback Method
cpg	1409.86	J/mol×K	1245.85	Joback Method
cpg	1418.89	J/mol×K	1288.30	Joback Method
cpg	1426.37	J/mol×K	1330.74	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=U376831&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