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

Inchi: InChI=1S/C28H43BrF2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-34-27(32)17-16-18-
InchiKey: IXLBYCHIDJSIEO-UHFFFAOYSA-N
Formula: C28H43BrF2O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 561.54

Physical Properties

Property code	Value	Unit	Source
gf	-574.74	kJ/mol	Joback Method
hf	-1274.62	kJ/mol	Joback Method
hfus	78.17	kJ/mol	Joback Method
hvap	105.30	kJ/mol	Joback Method
log10ws	-10.69		Crippen Method
logp	8.965		Crippen Method
mcvol	417.540	ml/mol	McGowan Method
pc	793.94	kPa	Joback Method
rinpol	3521.00		NIST Webbook
rinpol	3521.00		NIST Webbook
tb	1098.94	K	Joback Method
tc	1365.42	K	Joback Method
tf	674.60	K	Joback Method
vc	1.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1419.07	J/mol×K	1098.94	Joback Method
cpg	1435.55	J/mol×K	1143.35	Joback Method
cpg	1449.96	J/mol×K	1187.77	Joback Method
cpg	1462.42	J/mol×K	1232.18	Joback Method
cpg	1473.03	J/mol×K	1276.59	Joback Method
cpg	1481.88	J/mol×K	1321.00	Joback Method
cpg	1489.07	J/mol×K	1365.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376832&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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