Glutaric acid, 2-bromo-5-fluorobenzyl heptadecyl ester

Inchi: InChI=1S/C29H46BrFO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-34-28(32)18-17-1

InchiKey: XCNVNCHXGHMVHM-UHFFFAOYSA-N

Formula: C29H46BrFO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 557.58

Physical Properties

Property code	Value	Unit	Source
gf	-361.88	kJ/mol	Joback Method
hf	-1087.68	kJ/mol	Joback Method
hfus	78.07	kJ/mol	Joback Method
hvap	107.68	kJ/mol	Joback Method
log10ws	-10.78		Crippen Method
logp	9.216		Crippen Method
mcvol	429.860	ml/mol	McGowan Method
pc	778.08	kPa	Joback Method
rinpol	3659.00		NIST Webbook
tb	1117.57	K	Joback Method
tc	1389.21	K	Joback Method
tf	672.76	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1476.78	J/mol×K	1117.57	Joback Method
cpg	1493.78	J/mol×K	1162.84	Joback Method
cpg	1508.71	J/mol×K	1208.12	Joback Method
cpg	1521.69	J/mol×K	1253.39	Joback Method
cpg	1532.84	J/mol×K	1298.66	Joback Method
cpg	1542.29	J/mol×K	1343.94	Joback Method
cpg	1550.15	J/mol×K	1389.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376865&Units=SI

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

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