Glutaric acid, 2,5-difluorobenzyl eicosyl ester

Inchi: InChI=1S/C32H52F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-25-37-31(35
InchiKey: RDDAJRSVWVIRPW-UHFFFAOYSA-N
Formula: C32H52F2O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 538.75

Physical Properties

Property code	Value	Unit	Source
gf	-545.75	kJ/mol	Joback Method
hf	-1372.04	kJ/mol	Joback Method
hfus	83.63	kJ/mol	Joback Method
hvap	107.10	kJ/mol	Joback Method
log10ws	-11.20		Crippen Method
logp	9.763		Crippen Method
mcvol	456.400	ml/mol	McGowan Method
pc	629.08	kPa	Joback Method
rinpol	3681.00		NIST Webbook
rinpol	3681.00		NIST Webbook
tb	1119.32	K	Joback Method
tc	1417.97	K	Joback Method
tf	647.36	K	Joback Method
vc	1.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1636.64	J/mol×K	1119.32	Joback Method
cpg	1657.08	J/mol×K	1169.09	Joback Method
cpg	1674.63	J/mol×K	1218.87	Joback Method
cpg	1689.45	J/mol×K	1268.64	Joback Method
cpg	1701.71	J/mol×K	1318.42	Joback Method
cpg	1711.57	J/mol×K	1368.19	Joback Method
cpg	1719.22	J/mol×K	1417.97	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=U376961&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