Glutaric acid, octadecyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C30H47F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-36-28(34)19-18

InchiKey: NCTIEFDHYZZYJX-UHFFFAOYSA-N

Formula: C30H47F3O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 528.69

Physical Properties

Property code	Value	Unit	Source
gf	-767.03	kJ/mol	Joback Method
hf	-1538.34	kJ/mol	Joback Method
hfus	81.14	kJ/mol	Joback Method
hvap	102.50	kJ/mol	Joback Method
log10ws	-10.70		Crippen Method
logp	9.122		Crippen Method
mcvol	429.990	ml/mol	McGowan Method
pc	672.90	kPa	Joback Method
rinpol	3471.00		NIST Webbook
rinpol	3471.00		NIST Webbook
tb	1077.81	K	Joback Method
tc	1354.40	K	Joback Method
tf	637.93	K	Joback Method
vc	1.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1514.51	J/mol×K	1077.81	Joback Method
cpg	1533.92	J/mol×K	1123.91	Joback Method
cpg	1550.76	J/mol×K	1170.01	Joback Method
cpg	1565.15	J/mol×K	1216.11	Joback Method
cpg	1577.21	J/mol×K	1262.21	Joback Method
cpg	1587.03	J/mol×K	1308.31	Joback Method
cpg	1594.73	J/mol×K	1354.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376910&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

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