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

Inchi: InChI=1S/C27H41F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-33-25(31)16-15-17-26(32
InchiKey: LGSALPVTKPQNJT-UHFFFAOYSA-N
Formula: C27H41F3O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 486.61

Physical Properties

Property code	Value	Unit	Source
gf	-792.29	kJ/mol	Joback Method
hf	-1476.42	kJ/mol	Joback Method
hfus	73.37	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	7.952		Crippen Method
mcvol	387.720	ml/mol	McGowan Method
pc	785.95	kPa	Joback Method
rinpol	3161.00		NIST Webbook
rinpol	3161.00		NIST Webbook
tb	1009.17	K	Joback Method
tc	1247.41	K	Joback Method
tf	604.12	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1325.28	J/mol×K	1009.17	Joback Method
cpg	1343.13	J/mol×K	1048.88	Joback Method
cpg	1359.11	J/mol×K	1088.58	Joback Method
cpg	1373.27	J/mol×K	1128.29	Joback Method
cpg	1385.68	J/mol×K	1168.00	Joback Method
cpg	1396.39	J/mol×K	1207.71	Joback Method
cpg	1405.45	J/mol×K	1247.41	Joback Method

Sources

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=U376907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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