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

Inchi: InChI=1S/C29H45F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-35-27(33)18-17-19
InchiKey: LUNLSADBXGYOIR-UHFFFAOYSA-N
Formula: C29H45F3O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 514.66

Physical Properties

Property code	Value	Unit	Source
gf	-775.45	kJ/mol	Joback Method
hf	-1517.70	kJ/mol	Joback Method
hfus	78.55	kJ/mol	Joback Method
hvap	100.27	kJ/mol	Joback Method
log10ws	-10.28		Crippen Method
logp	8.732		Crippen Method
mcvol	415.900	ml/mol	McGowan Method
pc	707.71	kPa	Joback Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook
tb	1054.93	K	Joback Method
tc	1317.17	K	Joback Method
tf	626.66	K	Joback Method
vc	1.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1451.16	J/mol×K	1054.93	Joback Method
cpg	1470.02	J/mol×K	1098.64	Joback Method
cpg	1486.59	J/mol×K	1142.34	Joback Method
cpg	1500.94	J/mol×K	1186.05	Joback Method
cpg	1513.18	J/mol×K	1229.76	Joback Method
cpg	1523.38	J/mol×K	1273.47	Joback Method
cpg	1531.64	J/mol×K	1317.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376909&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