Glutaric acid, tetradecyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C27H41F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-21-33-25(31)15-14-16-26(32)34
InchiKey: FBZPIWQUELOTPV-UHFFFAOYSA-N
Formula: C27H41F3O5
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 502.61

Physical Properties

Property code	Value	Unit	Source
gf	-875.19	kJ/mol	Joback Method
hf	-1594.45	kJ/mol	Joback Method
hfus	67.93	kJ/mol	Joback Method
hvap	95.61	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.043		Crippen Method
mcvol	393.590	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	1018.40	K	Joback Method
tc	1256.83	K	Joback Method
tf	603.73	K	Joback Method
vc	1.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.51	J/mol×K	1018.40	Joback Method
cpg	1372.67	J/mol×K	1058.14	Joback Method
cpg	1388.02	J/mol×K	1097.88	Joback Method
cpg	1401.65	J/mol×K	1137.61	Joback Method
cpg	1413.63	J/mol×K	1177.35	Joback Method
cpg	1424.06	J/mol×K	1217.09	Joback Method
cpg	1433.02	J/mol×K	1256.83	Joback Method

Sources

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=U377345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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