Glutaric acid, 4-(trifluoromethoxy)benzyl undecyl ester

Inchi: InChI=1S/C24H35F3O5/c1-2-3-4-5-6-7-8-9-10-18-30-22(28)12-11-13-23(29)31-19-20-14

InchiKey: CHEUWTNBUAKENO-UHFFFAOYSA-N

Formula: C24H35F3O5

SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 460.53

Physical Properties

Property code	Value	Unit	Source
gf	-900.45	kJ/mol	Joback Method
hf	-1532.53	kJ/mol	Joback Method
hfus	60.16	kJ/mol	Joback Method
hvap	88.93	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	6.873		Crippen Method
mcvol	351.320	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
tb	949.76	K	Joback Method
tc	1163.59	K	Joback Method
tf	569.92	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.07	J/mol×K	949.76	Joback Method
cpg	1186.04	J/mol×K	985.40	Joback Method
cpg	1200.58	J/mol×K	1021.04	Joback Method
cpg	1213.75	J/mol×K	1056.68	Joback Method
cpg	1225.59	J/mol×K	1092.32	Joback Method
cpg	1236.15	J/mol×K	1127.95	Joback Method
cpg	1245.49	J/mol×K	1163.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377342&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