Glutaric acid, heptadecyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C30H47F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-24-36-28(34)18-17-19

InchiKey: KZIDRPPOPPJNRU-UHFFFAOYSA-N

Formula: C30H47F3O5

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

Mol. weight [g/mol]: 544.69

Physical Properties

Property code	Value	Unit	Source
gf	-849.93	kJ/mol	Joback Method
hf	-1656.37	kJ/mol	Joback Method
hfus	75.70	kJ/mol	Joback Method
hvap	102.29	kJ/mol	Joback Method
log10ws	-10.56		Crippen Method
logp	9.213		Crippen Method
mcvol	435.860	ml/mol	McGowan Method
pc	684.21	kPa	Joback Method
rinpol	3378.00		NIST Webbook
tb	1087.04	K	Joback Method
tc	1362.33	K	Joback Method
tf	637.54	K	Joback Method
vc	1.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1544.10	J/mol×K	1087.04	Joback Method
cpg	1562.72	J/mol×K	1132.92	Joback Method
cpg	1578.97	J/mol×K	1178.80	Joback Method
cpg	1592.99	J/mol×K	1224.68	Joback Method
cpg	1604.93	J/mol×K	1270.57	Joback Method
cpg	1614.93	J/mol×K	1316.45	Joback Method
cpg	1623.14	J/mol×K	1362.33	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=U377348&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