Glutaric acid, hexadecyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C29H45F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-23-35-27(33)17-16-18-28

InchiKey: RUUNUMIBMNPKQX-UHFFFAOYSA-N

Formula: C29H45F3O5

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

Mol. weight [g/mol]: 530.66

Physical Properties

Property code	Value	Unit	Source
gf	-858.35	kJ/mol	Joback Method
hf	-1635.73	kJ/mol	Joback Method
hfus	73.11	kJ/mol	Joback Method
hvap	100.06	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	8.823		Crippen Method
mcvol	421.770	ml/mol	McGowan Method
pc	719.91	kPa	Joback Method
rinpol	3278.00		NIST Webbook
rinpol	3278.00		NIST Webbook
tb	1064.16	K	Joback Method
tc	1325.62	K	Joback Method
tf	626.27	K	Joback Method
vc	1.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.95	J/mol×K	1064.16	Joback Method
cpg	1499.05	J/mol×K	1107.74	Joback Method
cpg	1515.00	J/mol×K	1151.31	Joback Method
cpg	1528.90	J/mol×K	1194.89	Joback Method
cpg	1540.88	J/mol×K	1238.47	Joback Method
cpg	1551.06	J/mol×K	1282.04	Joback Method
cpg	1559.56	J/mol×K	1325.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377347&Units=SI

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