

Glutaric acid, monoamide, N-(3,5-di(trifluoromethyl)benzyl)-, octadecyl

Inchi:
ester

InChI=1S/C32H49F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-42-30(41)20-1

InchiKey:

IYHLWWWOLUDZEY-UHFFFAOYSA-N

Formula:

C32H49F6NO3

SMILES:

CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1

Mol. weight [g/mol]:

609.73

Physical Properties

Property code	Value	Unit	Source
gf	-1124.92	kJ/mol	Joback Method
hf	-1988.29	kJ/mol	Joback Method
hfus	85.04	kJ/mol	Joback Method
hvap	105.27	kJ/mol	Joback Method
log10ws	-12.01		Crippen Method
logp	10.315		Crippen Method
mvol	467.590	ml/mol	McGowan Method
pc	595.17	kPa	Joback Method
rinpol	3476.00		NIST Webbook
rinpol	3476.00		NIST Webbook
tb	1137.69	K	Joback Method
tc	1463.30	K	Joback Method
tf	684.99	K	Joback Method
vc	1.871	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1696.45	J/molxK	1137.69	Joback Method
cpg	1720.43	J/molxK	1191.96	Joback Method
cpg	1742.58	J/molxK	1246.23	Joback Method
cpg	1763.34	J/molxK	1300.49	Joback Method
cpg	1783.16	J/molxK	1354.76	Joback Method
cpg	1802.48	J/molxK	1409.03	Joback Method
cpg	1821.73	J/molxK	1463.30	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=U360777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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