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

Inchi: InChI=1S/C30H45F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-40-28(39)18-16-17-2
InchiKey: YBVRBHPRQHDVOU-UHFFFAOYSA-N
Formula: C30H45F6NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 581.67

Physical Properties

Property code	Value	Unit	Source
gf	-1141.76	kJ/mol	Joback Method
hf	-1947.01	kJ/mol	Joback Method
hfus	79.86	kJ/mol	Joback Method
hvap	100.82	kJ/mol	Joback Method
log10ws	-11.18		Crippen Method
logp	9.535		Crippen Method
mcvol	439.410	ml/mol	McGowan Method
pc	655.11	kPa	Joback Method
rinpol	3264.00		NIST Webbook
tb	1091.93	K	Joback Method
tc	1380.36	K	Joback Method
tf	662.45	K	Joback Method
vc	1.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1567.58	J/mol×K	1091.93	Joback Method
cpg	1588.87	J/mol×K	1140.00	Joback Method
cpg	1608.52	J/mol×K	1188.07	Joback Method
cpg	1626.83	J/mol×K	1236.15	Joback Method
cpg	1644.08	J/mol×K	1284.22	Joback Method
cpg	1660.56	J/mol×K	1332.29	Joback Method
cpg	1676.57	J/mol×K	1380.36	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=U360776&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