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

Inchi: InChI=1S/C25H35F6NO3/c1-2-3-4-5-6-7-8-9-10-14-35-23(34)13-11-12-22(33)32-18-19-1

InchiKey: JIKSORHWBCNMMQ-UHFFFAOYSA-N

Formula: C25H35F6NO3

SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 511.54

Physical Properties

Property code	Value	Unit	Source
gf	-1183.86	kJ/mol	Joback Method
hf	-1843.81	kJ/mol	Joback Method
hfus	66.91	kJ/mol	Joback Method
hvap	89.69	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	7.585		Crippen Method
mcvol	368.960	ml/mol	McGowan Method
pc	851.47	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	977.53	K	Joback Method
tc	1203.19	K	Joback Method
tf	606.10	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.16	J/mol×K	977.53	Joback Method
cpg	1269.85	J/mol×K	1015.14	Joback Method
cpg	1285.33	J/mol×K	1052.75	Joback Method
cpg	1299.72	J/mol×K	1090.36	Joback Method
cpg	1313.15	J/mol×K	1127.97	Joback Method
cpg	1325.72	J/mol×K	1165.58	Joback Method
cpg	1337.57	J/mol×K	1203.19	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=U360772&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