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

Inchi: InChI=1S/C22H29F6NO3/c1-2-3-4-5-6-7-11-32-20(31)10-8-9-19(30)29-15-16-12-17(21(2

InchiKey: VTWSZMCDPRDEOK-UHFFFAOYSA-N

Formula: C22H29F6NO3

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

Mol. weight [g/mol]: 469.46

Physical Properties

Property code	Value	Unit	Source
gf	-1209.12	kJ/mol	Joback Method
hf	-1781.89	kJ/mol	Joback Method
hfus	59.14	kJ/mol	Joback Method
hvap	83.01	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	6.414		Crippen Method
mcvol	326.690	ml/mol	McGowan Method
pc	1014.89	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	908.89	K	Joback Method
tc	1112.85	K	Joback Method
tf	572.29	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.90	J/mol×K	908.89	Joback Method
cpg	1085.78	J/mol×K	942.88	Joback Method
cpg	1099.64	J/mol×K	976.88	Joback Method
cpg	1112.54	J/mol×K	1010.87	Joback Method
cpg	1124.57	J/mol×K	1044.87	Joback Method
cpg	1135.81	J/mol×K	1078.86	Joback Method
cpg	1146.34	J/mol×K	1112.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360770&Units=SI
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

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