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

Inchi: InChI=1S/C21H27F6NO3/c1-2-3-4-5-6-10-31-19(30)9-7-8-18(29)28-14-15-11-16(20(22,2

InchiKey: TVXDZLVUAQGOES-UHFFFAOYSA-N

Formula: C21H27F6NO3

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

Mol. weight [g/mol]: 455.43

Physical Properties

Property code	Value	Unit	Source
gf	-1217.54	kJ/mol	Joback Method
hf	-1761.25	kJ/mol	Joback Method
hfus	56.55	kJ/mol	Joback Method
hvap	80.78	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.024		Crippen Method
mcvol	312.600	ml/mol	McGowan Method
pc	1079.93	kPa	Joback Method
rinpol	2402.00		NIST Webbook
tb	886.01	K	Joback Method
tc	1084.85	K	Joback Method
tf	561.02	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.42	J/mol×K	886.01	Joback Method
cpg	1025.81	J/mol×K	919.15	Joback Method
cpg	1039.21	J/mol×K	952.29	Joback Method
cpg	1051.70	J/mol×K	985.43	Joback Method
cpg	1063.34	J/mol×K	1018.57	Joback Method
cpg	1074.22	J/mol×K	1051.71	Joback Method
cpg	1084.39	J/mol×K	1084.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360769&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