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

Inchi: InChI=1S/C24H33F6NO3/c1-2-3-4-5-6-7-8-9-13-34-22(33)12-10-11-21(32)31-17-18-14-1

InchiKey: QMBRHDUTTTWWSF-UHFFFAOYSA-N

Formula: C24H33F6NO3

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

Mol. weight [g/mol]: 497.51

Physical Properties

Property code	Value	Unit	Source
gf	-1192.28	kJ/mol	Joback Method
hf	-1823.17	kJ/mol	Joback Method
hfus	64.32	kJ/mol	Joback Method
hvap	87.46	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.195		Crippen Method
mcvol	354.870	ml/mol	McGowan Method
pc	901.26	kPa	Joback Method
rinpol	2677.00		NIST Webbook
rinpol	2677.00		NIST Webbook
tb	954.65	K	Joback Method
tc	1171.94	K	Joback Method
tf	594.83	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.81	J/mol×K	954.65	Joback Method
cpg	1207.83	J/mol×K	990.87	Joback Method
cpg	1222.72	J/mol×K	1027.08	Joback Method
cpg	1236.57	J/mol×K	1063.30	Joback Method
cpg	1249.48	J/mol×K	1099.51	Joback Method
cpg	1261.56	J/mol×K	1135.73	Joback Method
cpg	1272.91	J/mol×K	1171.94	Joback Method

Sources

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=U360771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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