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

Inchi: InChI=1S/C19H23F6NO3/c1-2-3-4-8-29-17(28)7-5-6-16(27)26-12-13-9-14(18(20,21)22)1

InchiKey: DTEJEGDCCCUNTL-UHFFFAOYSA-N

Formula: C19H23F6NO3

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

Mol. weight [g/mol]: 427.38

Physical Properties

Property code	Value	Unit	Source
gf	-1234.38	kJ/mol	Joback Method
hf	-1719.97	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	76.33	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.244		Crippen Method
mcvol	284.420	ml/mol	McGowan Method
pc	1230.28	kPa	Joback Method
rinpol	2219.00		NIST Webbook
tb	840.25	K	Joback Method
tc	1031.54	K	Joback Method
tf	538.48	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.66	J/mol×K	840.25	Joback Method
cpg	908.16	J/mol×K	872.13	Joback Method
cpg	920.75	J/mol×K	904.01	Joback Method
cpg	932.49	J/mol×K	935.89	Joback Method
cpg	943.43	J/mol×K	967.78	Joback Method
cpg	953.63	J/mol×K	999.66	Joback Method
cpg	963.16	J/mol×K	1031.54	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=U360767&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