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

Inchi: InChI=1S/C17H19F6NO3/c1-2-6-27-15(26)5-3-4-14(25)24-10-11-7-12(16(18,19)20)9-13(

InchiKey: CTHYLPKCJVEDIB-UHFFFAOYSA-N

Formula: C17H19F6NO3

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

Mol. weight [g/mol]: 399.33

Physical Properties

Property code	Value	Unit	Source
gf	-1251.22	kJ/mol	Joback Method
hf	-1678.69	kJ/mol	Joback Method
hfus	46.19	kJ/mol	Joback Method
hvap	71.88	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.464		Crippen Method
mcvol	256.240	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook
tb	794.49	K	Joback Method
tc	981.40	K	Joback Method
tf	515.94	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.17	J/mol×K	794.49	Joback Method
cpg	793.87	J/mol×K	825.64	Joback Method
cpg	805.71	J/mol×K	856.79	Joback Method
cpg	816.75	J/mol×K	887.95	Joback Method
cpg	827.03	J/mol×K	919.10	Joback Method
cpg	836.60	J/mol×K	950.25	Joback Method
cpg	845.52	J/mol×K	981.40	Joback Method

Sources

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=U360764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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