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

Inchi: InChI=1S/C18H21F6NO3/c1-2-3-7-28-16(27)6-4-5-15(26)25-11-12-8-13(17(19,20)21)10-

InchiKey: LWQJZXFESBMKRV-UHFFFAOYSA-N

Formula: C18H21F6NO3

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

Mol. weight [g/mol]: 413.35

Physical Properties

Property code	Value	Unit	Source
gf	-1242.80	kJ/mol	Joback Method
hf	-1699.33	kJ/mol	Joback Method
hfus	48.78	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.854		Crippen Method
mcvol	270.330	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2129.00		NIST Webbook
tb	817.37	K	Joback Method
tc	1006.10	K	Joback Method
tf	527.21	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.48	J/mol×K	817.37	Joback Method
cpg	850.57	J/mol×K	848.83	Joback Method
cpg	862.78	J/mol×K	880.28	Joback Method
cpg	874.17	J/mol×K	911.74	Joback Method
cpg	884.78	J/mol×K	943.19	Joback Method
cpg	894.66	J/mol×K	974.65	Joback Method
cpg	903.89	J/mol×K	1006.10	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=U360766&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