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

Inchi: InChI=1S/C18H21F6NO3/c1-11(2)10-28-16(27)5-3-4-15(26)25-9-12-6-13(17(19,20)21)8-

InchiKey: OGYPGGLCWDVDBX-UHFFFAOYSA-N

Formula: C18H21F6NO3

SMILES: CC(C)COC(=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	-1245.24	kJ/mol	Joback Method
hf	-1704.61	kJ/mol	Joback Method
hfus	45.25	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.710		Crippen Method
mcvol	270.330	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
tb	816.93	K	Joback Method
tc	1006.83	K	Joback Method
tf	512.21	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.03	J/mol×K	816.93	Joback Method
cpg	851.21	J/mol×K	848.58	Joback Method
cpg	863.47	J/mol×K	880.23	Joback Method
cpg	874.89	J/mol×K	911.88	Joback Method
cpg	885.52	J/mol×K	943.53	Joback Method
cpg	895.41	J/mol×K	975.18	Joback Method
cpg	904.62	J/mol×K	1006.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360765&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

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