Glutaric acid, diamide, N,N'-di(3,5-di(trifluoromethyl)benzyl)-

Inchi: InChI=1S/C23H18F12N2O2/c24-20(25,26)14-4-12(5-15(8-14)21(27,28)29)10-36-18(38)2

InchiKey: JEHPUGXIKMXUCP-UHFFFAOYSA-N

Formula: C23H18F12N2O2

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

Mol. weight [g/mol]: 582.38

Physical Properties

Property code	Value	Unit	Source
gf	-2076.34	kJ/mol	Joback Method
hf	-2597.41	kJ/mol	Joback Method
hfus	62.55	kJ/mol	Joback Method
hvap	85.37	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	6.865		Crippen Method
mcvol	331.750	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2599.00		NIST Webbook
rinpol	2599.00		NIST Webbook
tb	985.32	K	Joback Method
tc	1208.92	K	Joback Method
tf	673.83	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.52	J/mol×K	985.32	Joback Method
cpg	1106.31	J/mol×K	1022.59	Joback Method
cpg	1117.51	J/mol×K	1059.85	Joback Method
cpg	1128.31	J/mol×K	1097.12	Joback Method
cpg	1138.87	J/mol×K	1134.39	Joback Method
cpg	1149.37	J/mol×K	1171.65	Joback Method
cpg	1159.99	J/mol×K	1208.92	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=U360778&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