Glutaric acid, monoamide, N,N-di(4-methylphenyl)-, isobutyl ester

Inchi: InChI=1S/C23H29NO3/c1-17(2)16-27-23(26)7-5-6-22(25)24(20-12-8-18(3)9-13-20)21-14

InchiKey: NLOCCALFVHBTED-UHFFFAOYSA-N

Formula: C23H29NO3

SMILES: Cc1ccc(N(C(=O)CCCC(=O)OCC(C)C)c2ccc(C)cc2)cc1

Mol. weight [g/mol]: 367.48

Physical Properties

Property code	Value	Unit	Source
gf	93.84	kJ/mol	Joback Method
hf	-363.06	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.338		Crippen Method
mcvol	306.400	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2746.00		NIST Webbook
rinpol	2746.00		NIST Webbook
tb	931.12	K	Joback Method
tc	1154.54	K	Joback Method
tf	566.41	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.96	J/mol×K	931.12	Joback Method
cpg	986.07	J/mol×K	968.36	Joback Method
cpg	999.89	J/mol×K	1005.59	Joback Method
cpg	1012.51	J/mol×K	1042.83	Joback Method
cpg	1023.98	J/mol×K	1080.07	Joback Method
cpg	1034.39	J/mol×K	1117.31	Joback Method
cpg	1043.80	J/mol×K	1154.54	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=U360231&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