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

Inchi: InChI=1S/C23H29NO3/c1-4-5-17-27-23(26)8-6-7-22(25)24(20-13-9-18(2)10-14-20)21-15

InchiKey: JHZHXVTXNOCJNI-UHFFFAOYSA-N

Formula: C23H29NO3

SMILES: CCCCOC(=O)CCCC(=O)N(c1ccc(C)cc1)c1ccc(C)cc1

Mol. weight [g/mol]: 367.48

Physical Properties

Property code	Value	Unit	Source
gf	96.28	kJ/mol	Joback Method
hf	-357.78	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	90.61	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.482		Crippen Method
mcvol	306.400	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2793.00		NIST Webbook
tb	931.56	K	Joback Method
tc	1153.04	K	Joback Method
tf	581.41	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.50	J/mol×K	931.56	Joback Method
cpg	985.52	J/mol×K	968.47	Joback Method
cpg	999.29	J/mol×K	1005.39	Joback Method
cpg	1011.89	J/mol×K	1042.30	Joback Method
cpg	1023.38	J/mol×K	1079.22	Joback Method
cpg	1033.83	J/mol×K	1116.13	Joback Method
cpg	1043.32	J/mol×K	1153.04	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=U360232&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

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