Glutaric acid, monoamide, N-butyl-N-phenyl-, octyl ester

Inchi: InChI=1S/C23H37NO3/c1-3-5-7-8-9-13-20-27-23(26)18-14-17-22(25)24(19-6-4-2)21-15-
InchiKey: PGKOSLFQBYBWRC-UHFFFAOYSA-N
Formula: C23H37NO3
SMILES: CCCCCCCCOC(=O)CCCC(=O)N(CCCC)c1ccccc1
Mol. weight [g/mol]: 375.54

Physical Properties

Property code	Value	Unit	Source
gf	3.13	kJ/mol	Joback Method
hf	-571.37	kJ/mol	Joback Method
hfus	56.77	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.894		Crippen Method
mcvol	330.160	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2731.00		NIST Webbook
tb	894.92	K	Joback Method
tc	1098.19	K	Joback Method
tf	529.95	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1071.71	J/mol×K	894.92	Joback Method
cpg	1089.14	J/mol×K	928.80	Joback Method
cpg	1105.38	J/mol×K	962.68	Joback Method
cpg	1120.49	J/mol×K	996.55	Joback Method
cpg	1134.52	J/mol×K	1030.43	Joback Method
cpg	1147.54	J/mol×K	1064.31	Joback Method
cpg	1159.60	J/mol×K	1098.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360177&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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