

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

Inchi: InChI=1S/C25H41NO3/c1-3-5-7-8-9-10-11-15-22-29-25(28)20-16-19-24(27)26(21-6-4-2)
InchiKey: IBVMFJAEXXGUHJ-UHFFFAOYSA-N
Formula: C25H41NO3
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)N(CCCC)c1ccccc1
Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
gf	19.97	kJ/mol	Joback Method
hf	-612.65	kJ/mol	Joback Method
hfus	61.95	kJ/mol	Joback Method
hvap	91.46	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.674		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2948.00		NIST Webbook
tb	940.68	K	Joback Method
tc	1151.70	K	Joback Method
tf	552.49	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.41	J/mol×K	940.68	Joback Method
cpg	1213.49	J/mol×K	975.85	Joback Method
cpg	1230.27	J/mol×K	1011.02	Joback Method
cpg	1245.83	J/mol×K	1046.19	Joback Method
cpg	1260.24	J/mol×K	1081.36	Joback Method
cpg	1273.57	J/mol×K	1116.53	Joback Method
cpg	1285.90	J/mol×K	1151.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U360179&Units=SI

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
hvac:	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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