Glutaric acid, monoamide, N-methyl-N-benzyl-, octyl ester

Inchi: InChI=1S/C21H33NO3/c1-3-4-5-6-7-11-17-25-21(24)16-12-15-20(23)22(2)18-19-13-9-8-
InchiKey: WSYUGFXQPRUZGJ-UHFFFAOYSA-N
Formula: C21H33NO3
SMILES: CCCCCCCCOC(=O)CCCC(=O)N(C)Cc1ccccc1
Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-13.71	kJ/mol	Joback Method
hf	-530.09	kJ/mol	Joback Method
hfus	51.59	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.719		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2771.00		NIST Webbook
tb	849.16	K	Joback Method
tc	1048.11	K	Joback Method
tf	507.41	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.52	J/mol×K	849.16	Joback Method
cpg	967.43	J/mol×K	882.32	Joback Method
cpg	983.23	J/mol×K	915.48	Joback Method
cpg	997.96	J/mol×K	948.64	Joback Method
cpg	1011.67	J/mol×K	981.79	Joback Method
cpg	1024.41	J/mol×K	1014.95	Joback Method
cpg	1036.23	J/mol×K	1048.11	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=U360843&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