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

Inchi: InChI=1S/C20H31NO3/c1-3-4-5-6-10-16-24-20(23)15-11-14-19(22)21(2)17-18-12-8-7-9-
InchiKey: LILVLIMWOPBRGN-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CCCCCCCOC(=O)CCCC(=O)N(C)Cc1ccccc1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-22.13	kJ/mol	Joback Method
hf	-509.45	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.329		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	2648.00		NIST Webbook
rinpol	2648.00		NIST Webbook
tb	826.28	K	Joback Method
tc	1024.21	K	Joback Method
tf	496.14	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.01	J/mol×K	826.28	Joback Method
cpg	907.69	J/mol×K	859.27	Joback Method
cpg	923.29	J/mol×K	892.26	Joback Method
cpg	937.83	J/mol×K	925.25	Joback Method
cpg	951.39	J/mol×K	958.24	Joback Method
cpg	963.99	J/mol×K	991.22	Joback Method
cpg	975.69	J/mol×K	1024.21	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=U360842&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

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