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

Inchi: InChI=1S/C28H47NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-24-32-28(31)23-19-22-27(30

InchiKey: WVZJGIFULZWVPM-UHFFFAOYSA-N

Formula: C28H47NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCC(=O)N(C)Cc1ccccc1

Mol. weight [g/mol]: 445.68

Physical Properties

Property code	Value	Unit	Source
gf	45.23	kJ/mol	Joback Method
hf	-674.57	kJ/mol	Joback Method
hfus	69.72	kJ/mol	Joback Method
hvap	98.14	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.450		Crippen Method
mcvol	400.610	ml/mol	McGowan Method
pc	831.46	kPa	Joback Method
rinpol	3495.00		NIST Webbook
tb	1009.32	K	Joback Method
tc	1239.62	K	Joback Method
tf	586.30	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.87	J/mol×K	1009.32	Joback Method
cpg	1404.25	J/mol×K	1047.70	Joback Method
cpg	1422.13	J/mol×K	1086.09	Joback Method
cpg	1438.59	J/mol×K	1124.47	Joback Method
cpg	1453.75	J/mol×K	1162.86	Joback Method
cpg	1467.72	J/mol×K	1201.24	Joback Method
cpg	1480.59	J/mol×K	1239.62	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=U360848&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