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

Inchi: InChI=1S/C22H35NO3/c1-3-5-7-8-12-19-26-22(25)17-13-16-21(24)23(18-6-4-2)20-14-10

InchiKey: HHXVMJSUBWWTIC-UHFFFAOYSA-N

Formula: C22H35NO3

SMILES: CCCCCCCOC(=O)CCCC(=O)N(CCCC)c1ccccc1

Mol. weight [g/mol]: 361.52

Physical Properties

Property code	Value	Unit	Source
gf	-5.29	kJ/mol	Joback Method
hf	-550.73	kJ/mol	Joback Method
hfus	54.18	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.504		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook
tb	872.04	K	Joback Method
tc	1072.75	K	Joback Method
tf	518.68	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.77	J/mol×K	872.04	Joback Method
cpg	1027.93	J/mol×K	905.49	Joback Method
cpg	1043.94	J/mol×K	938.94	Joback Method
cpg	1058.86	J/mol×K	972.40	Joback Method
cpg	1072.72	J/mol×K	1005.85	Joback Method
cpg	1085.60	J/mol×K	1039.30	Joback Method
cpg	1097.54	J/mol×K	1072.75	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=U360176&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