Glutaric acid, monoamide, N-(1-phenylethyl)-, heptyl ester

Inchi: InChI=1S/C20H31NO3/c1-3-4-5-6-10-16-24-20(23)15-11-14-19(22)21-17(2)18-12-8-7-9-
InchiKey: XVMGJKWVGBSTIW-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-45.96	kJ/mol	Joback Method
hf	-528.79	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.548		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	2615.00		NIST Webbook
tb	863.57	K	Joback Method
tc	1067.89	K	Joback Method
tf	501.33	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.18	J/mol×K	863.57	Joback Method
cpg	925.17	J/mol×K	897.62	Joback Method
cpg	940.02	J/mol×K	931.68	Joback Method
cpg	953.79	J/mol×K	965.73	Joback Method
cpg	966.51	J/mol×K	999.78	Joback Method
cpg	978.23	J/mol×K	1033.84	Joback Method
cpg	989.00	J/mol×K	1067.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U360157&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
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