Glutaric acid, monoamide, N-(2-phenylpropyl)-, isohexyl ester

Inchi: InChI=1S/C20H31NO3/c1-16(2)9-8-14-24-20(23)13-7-12-19(22)21-15-17(3)18-10-5-4-6-
InchiKey: XFFQHLXQAIIBOD-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CC(C)CCCOC(=O)CCCC(=O)NCC(C)c1ccccc1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-48.40	kJ/mol	Joback Method
hf	-534.07	kJ/mol	Joback Method
hfus	44.04	kJ/mol	Joback Method
hvap	83.95	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.056		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2592.00		NIST Webbook
tb	863.13	K	Joback Method
tc	1069.16	K	Joback Method
tf	486.33	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.69	J/mol×K	863.13	Joback Method
cpg	925.79	J/mol×K	897.47	Joback Method
cpg	940.73	J/mol×K	931.81	Joback Method
cpg	954.55	J/mol×K	966.14	Joback Method
cpg	967.30	J/mol×K	1000.48	Joback Method
cpg	979.02	J/mol×K	1034.82	Joback Method
cpg	989.76	J/mol×K	1069.16	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=U360823&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