

Glutaric acid, monoamide, N-(2-ethylphenyl)-, hexyl ester

Inchi: InChI=1S/C19H29NO3/c1-3-5-6-9-15-23-19(22)14-10-13-18(21)20-17-12-8-7-11-16(17)4
InchiKey: KRBWBFKBYMQGFW-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CCCCCCOC(=O)CCCC(=O)Nc1ccccc1CC
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-61.57	kJ/mol	Joback Method
hf	-514.34	kJ/mol	Joback Method
hfus	48.10	kJ/mol	Joback Method
hvap	83.16	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.481		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tb	846.11	K	Joback Method
tc	1048.85	K	Joback Method
tf	517.58	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.95	J/mol×K	846.11	Joback Method
cpg	864.52	J/mol×K	879.90	Joback Method
cpg	879.02	J/mol×K	913.69	Joback Method
cpg	892.47	J/mol×K	947.48	Joback Method
cpg	904.93	J/mol×K	981.27	Joback Method
cpg	916.42	J/mol×K	1015.06	Joback Method
cpg	926.98	J/mol×K	1048.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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