

Glutaric acid, monoamide, N-(2-methoxyphenyl)-, nonyl ester

Inchi: InChI=1S/C21H33NO4/c1-3-4-5-6-7-8-11-17-26-21(24)16-12-15-20(23)22-18-13-9-10-14
InchiKey: PEWJVYPZKJFMBF-UHFFFAOYSA-N
Formula: C21H33NO4
SMILES: CCCCCCCCCOC(=O)CCCC(=O)Nc1ccccc1OC
Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
gf	-149.73	kJ/mol	Joback Method
hf	-687.84	kJ/mol	Joback Method
hfus	54.47	kJ/mol	Joback Method
hvap	90.03	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.098		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook
tb	914.29	K	Joback Method
tc	1122.24	K	Joback Method
tf	562.35	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.02	J/mol×K	914.29	Joback Method
cpg	1012.54	J/mol×K	948.95	Joback Method
cpg	1026.79	J/mol×K	983.61	Joback Method
cpg	1039.81	J/mol×K	1018.27	Joback Method
cpg	1051.64	J/mol×K	1052.92	Joback Method
cpg	1062.30	J/mol×K	1087.58	Joback Method
cpg	1071.81	J/mol×K	1122.24	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=U360936&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
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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