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

Inchi: InChI=1S/C18H27NO4/c1-14(2)8-7-13-23-18(21)12-6-11-17(20)19-15-9-4-5-10-16(15)22

InchiKey: QMDFDMXDUSAXJK-UHFFFAOYSA-N

Formula: C18H27NO4

SMILES: COc1ccccc1NC(=O)CCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
gf	-177.43	kJ/mol	Joback Method
hf	-631.20	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	82.96	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.783		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2813.00		NIST Webbook
tb	845.21	K	Joback Method
tc	1050.30	K	Joback Method
tf	513.54	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.83	J/mol×K	845.21	Joback Method
cpg	834.84	J/mol×K	879.39	Joback Method
cpg	848.71	J/mol×K	913.57	Joback Method
cpg	861.47	J/mol×K	947.76	Joback Method
cpg	873.14	J/mol×K	981.94	Joback Method
cpg	883.73	J/mol×K	1016.12	Joback Method
cpg	893.27	J/mol×K	1050.30	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=U360932&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