Glutaric acid, monoamide, N-(2-(4-methoxyphenyl)ethyl)-, isohexyl ester

Inchi: InChI=1S/C20H31NO4/c1-16(2)6-5-15-25-20(23)8-4-7-19(22)21-14-13-17-9-11-18(24-3)

InchiKey: PJOSTKOKYWKNJZ-UHFFFAOYSA-N

Formula: C20H31NO4

SMILES: COc1ccc(CCNC(=O)CCCC(=O)OCCCC(C)C)cc1

Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
gf	-160.59	kJ/mol	Joback Method
hf	-672.48	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.504		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2832.00		NIST Webbook
rinpol	2832.00		NIST Webbook
tb	890.97	K	Joback Method
tc	1097.78	K	Joback Method
tf	536.08	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.60	J/mol×K	890.97	Joback Method
cpg	952.96	J/mol×K	925.44	Joback Method
cpg	967.11	J/mol×K	959.91	Joback Method
cpg	980.05	J/mol×K	994.38	Joback Method
cpg	991.82	J/mol×K	1028.85	Joback Method
cpg	1002.44	J/mol×K	1063.31	Joback Method
cpg	1011.95	J/mol×K	1097.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360221&Units=SI
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

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