Glutaric acid, monoamide, N,N-di(4-methylphenyl)-, isohexyl ester

Inchi: InChI=1S/C25H33NO3/c1-19(2)7-6-18-29-25(28)9-5-8-24(27)26(22-14-10-20(3)11-15-22
InchiKey: JTNBDXFHNKQMDY-UHFFFAOYSA-N
Formula: C25H33NO3
SMILES: Cc1ccc(N(C(=O)CCCC(=O)OCCCC(C)C)c2ccc(C)cc2)cc1
Mol. weight [g/mol]: 395.53

Physical Properties

Property code	Value	Unit	Source
gf	110.68	kJ/mol	Joback Method
hf	-404.34	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	94.68	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	6.118		Crippen Method
mcvol	334.580	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2968.00		NIST Webbook
rinpol	2968.00		NIST Webbook
tb	976.88	K	Joback Method
tc	1201.97	K	Joback Method
tf	588.95	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.49	J/mol×K	976.88	Joback Method
cpg	1106.78	J/mol×K	1014.39	Joback Method
cpg	1120.76	J/mol×K	1051.91	Joback Method
cpg	1133.51	J/mol×K	1089.42	Joback Method
cpg	1145.11	J/mol×K	1126.94	Joback Method
cpg	1155.62	J/mol×K	1164.45	Joback Method
cpg	1165.15	J/mol×K	1201.97	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=U360234&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