

Glutaric acid, isohexyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C24H30O5/c1-19(2)9-8-16-27-23(25)14-7-15-24(26)28-18-20-10-6-13-22(17-2
InchiKey:	YMFVYDUJXMLPNX-UHFFFAOYSA-N
Formula:	C24H30O5
SMILES:	CC(C)CCCOC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	398.49

Physical Properties

Property code	Value	Unit	Source
gf	-208.89	kJ/mol	Joback Method
hf	-704.20	kJ/mol	Joback Method
hfus	48.85	kJ/mol	Joback Method
hvap	94.57	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.672		Crippen Method
mcvol	322.250	ml/mol	McGowan Method
pc	1282.83	kPa	Joback Method
rinpola	3036.00		NIST Webbook
tb	981.42	K	Joback Method
tc	1207.31	K	Joback Method
tf	577.15	K	Joback Method
vc	1.224	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.62	J/molxK	981.42	Joback Method
cpg	1097.02	J/molxK	1169.66	Joback Method
cpg	1089.51	J/molxK	1132.01	Joback Method
cpg	1080.55	J/molxK	1094.36	Joback Method
cpg	1070.11	J/molxK	1056.72	Joback Method
cpg	1058.15	J/molxK	1019.07	Joback Method
cpg	1103.11	J/molxK	1207.31	Joback Method
dvisc	0.0000214	Paxs	981.42	Joback Method
dvisc	0.0000279	Paxs	914.04	Joback Method

dvisc	0.0000377	Paxs	846.66	Joback Method
dvisc	0.0000538	Paxs	779.28	Joback Method
dvisc	0.0000822	Paxs	711.91	Joback Method
dvisc	0.0001370	Paxs	644.53	Joback Method
dvisc	0.0002575	Paxs	577.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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