

Glutaric acid, isohexyl 3-phenylprop-2-enyl ester

Inchi:	InChI=1S/C20H28O4/c1-17(2)9-7-15-23-19(21)13-6-14-20(22)24-16-8-12-18-10-4-3-5-1
InchiKey:	RARGZJMXNPOUDS-XYOKQWHBSA-N
Formula:	C20H28O4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-160.13	kJ/mol	Joback Method
hf	-597.26	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.393		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpola	2575.00		NIST Webbook
tb	839.98	K	Joback Method
tc	1045.27	K	Joback Method
tf	465.82	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.53	J/molxK	839.98	Joback Method
cpg	868.41	J/molxK	874.19	Joback Method
cpg	883.19	J/molxK	908.41	Joback Method
cpg	896.90	J/molxK	942.62	Joback Method
cpg	909.59	J/molxK	976.84	Joback Method
cpg	921.29	J/molxK	1011.05	Joback Method
cpg	932.05	J/molxK	1045.27	Joback Method
dvisc	0.0007457	Paxs	465.82	Joback Method
dvisc	0.0003506	Paxs	528.18	Joback Method

dvisc	0.0001933	Paxs	590.54	Joback Method
dvisc	0.0001194	Paxs	652.90	Joback Method
dvisc	0.0000802	Paxs	715.26	Joback Method
dvisc	0.0000575	Paxs	777.62	Joback Method
dvisc	0.0000432	Paxs	839.98	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=U359890&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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