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

Inchi: InChI=1S/C20H28O4/c1-2-3-4-8-16-23-19(21)14-9-15-20(22)24-17-10-13-18-11-6-5-7-12
InchiKey: BZQLSNPIGQYAQL-JLHYYAGUSA-N
Formula: C20H28O4
SMILES: CCCCCCOC(=O)CCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-157.69	kJ/mol	Joback Method
hf	-591.98	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.537		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2615.00		NIST Webbook
tb	840.42	K	Joback Method
tc	1043.70	K	Joback Method
tf	480.82	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.00	J/mol×K	840.42	Joback Method
cpg	920.37	J/mol×K	1009.82	Joback Method
cpg	908.69	J/mol×K	975.94	Joback Method
cpg	896.05	J/mol×K	942.06	Joback Method
cpg	882.42	J/mol×K	908.18	Joback Method
cpg	867.75	J/mol×K	874.30	Joback Method
cpg	931.14	J/mol×K	1043.70	Joback Method
dvisc	0.0000472	Pa×s	840.42	Joback Method
dvisc	0.0000617	Pa×s	780.49	Joback Method

dvisc	0.0000844	Pa×s	720.55	Joback Method
dvisc	0.0001223	Pa×s	660.62	Joback Method
dvisc	0.0001906	Pa×s	600.69	Joback Method
dvisc	0.0003279	Pa×s	540.75	Joback Method
dvisc	0.0006456	Pa×s	480.82	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=U359891&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