Glutaric acid, cyclohexylmethyl 3-phenylpropyl ester

Inchi: InChI=1S/C21H30O4/c22-20(24-16-8-13-18-9-3-1-4-10-18)14-7-15-21(23)25-17-19-11-5

InchiKey: WWVWSHROGHQNJZ-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCCCc1ccccc1

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-205.04	kJ/mol	Joback Method
hf	-675.52	kJ/mol	Joback Method
hfus	41.60	kJ/mol	Joback Method
hvap	83.36	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.456		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	878.69	K	Joback Method
tc	1096.10	K	Joback Method
tf	504.55	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.14	J/mol×K	878.69	Joback Method
cpg	950.16	J/mol×K	914.92	Joback Method
cpg	965.69	J/mol×K	951.16	Joback Method
cpg	979.76	J/mol×K	987.39	Joback Method
cpg	992.42	J/mol×K	1023.63	Joback Method
cpg	1003.71	J/mol×K	1059.86	Joback Method
cpg	1013.66	J/mol×K	1096.10	Joback Method
dvisc	0.0007105	Pa×s	504.55	Joback Method

dvisc	0.0003551	Pa×s	566.91	Joback Method
dvisc	0.0002036	Pa×s	629.26	Joback Method
dvisc	0.0001290	Pa×s	691.62	Joback Method
dvisc	0.0000882	Pa×s	753.98	Joback Method
dvisc	0.0000639	Pa×s	816.33	Joback Method
dvisc	0.0000485	Pa×s	878.69	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=U391777&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