

Glutaric acid, cyclohexylmethyl phenethyl ester

Inchi:	InChI=1S/C20H28O4/c21-19(23-15-14-17-8-3-1-4-9-17)12-7-13-20(22)24-16-18-10-5-2-6
InchiKey:	OAEVBUGRPYRYSH-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	O=C(CCCC(=O)OCC1CCCCC1)OCCc1ccccc1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-213.46	kJ/mol	Joback Method
hf	-654.88	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	81.13	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.066		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinqol	2559.00		NIST Webbook
tb	855.81	K	Joback Method
tc	1074.27	K	Joback Method
tf	493.28	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.59	J/molxK	855.81	Joback Method
cpg	890.67	J/molxK	892.22	Joback Method
cpg	906.28	J/molxK	928.63	Joback Method
cpg	920.45	J/molxK	965.04	Joback Method
cpg	933.22	J/molxK	1001.45	Joback Method
cpg	944.62	J/molxK	1037.86	Joback Method
cpg	954.71	J/molxK	1074.27	Joback Method
dvisc	0.0007938	Paxs	493.28	Joback Method
dvisc	0.0004009	Paxs	553.70	Joback Method

dvisc	0.0002316	Paxs	614.12	Joback Method
dvisc	0.0001476	Paxs	674.54	Joback Method
dvisc	0.0001013	Paxs	734.97	Joback Method
dvisc	0.0000736	Paxs	795.39	Joback Method
dvisc	0.0000560	Paxs	855.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391792&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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