

Glutaric acid, 2-(cyclohexyl)ethyl cyclohexylmethyl ester

Inchi: InChI=1S/C20H34O4/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: XRMVSKNQTKFLIG-UHFFFAOYSA-N
Formula: C20H34O4
SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCCC1CCCCC1
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-301.42	kJ/mol	Joback Method
hf	-837.09	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.794		Crippen Method
mvol	285.820	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2506.00		NIST Webbook
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tb	848.68	K	Joback Method
tc	1062.77	K	Joback Method
tf	474.24	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.36	J/molxK	848.68	Joback Method
cpg	983.22	J/molxK	884.36	Joback Method
cpg	1001.42	J/molxK	920.04	Joback Method
cpg	1017.99	J/molxK	955.73	Joback Method
cpg	1032.97	J/molxK	991.41	Joback Method
cpg	1046.37	J/molxK	1027.09	Joback Method
cpg	1058.24	J/molxK	1062.77	Joback Method
dvisc	0.0010931	Paxs	474.24	Joback Method

dvisc	0.0005014	Paxs	536.65	Joback Method
dvisc	0.0002705	Paxs	599.05	Joback Method
dvisc	0.0001640	Paxs	661.46	Joback Method
dvisc	0.0001083	Paxs	723.87	Joback Method
dvisc	0.0000765	Paxs	786.27	Joback Method
dvisc	0.0000568	Paxs	848.68	Joback Method

Sources

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=U405421&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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