

1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl hexyl ester

Inchi:	InChI=1S/C21H36O4/c1-2-3-4-10-15-24-20(22)18-13-8-9-14-19(18)21(23)25-16-17-11-6
InchiKey:	SBPUMOMGRKKUAR-UHFFFAOYSA-N
Formula:	C21H36O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1
Mol. weight [g/mol]:	352.51

Physical Properties

Property code	Value	Unit	Source
gf	-300.71	kJ/mol	Joback Method
hf	-878.07	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	81.20	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.040		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	2498.00		NIST Webbook
tb	866.89	K	Joback Method
tc	1079.98	K	Joback Method
tf	481.27	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.27	J/molxK	866.89	Joback Method
cpg	1048.33	J/molxK	902.40	Joback Method
cpg	1066.65	J/molxK	937.92	Joback Method
cpg	1083.26	J/molxK	973.43	Joback Method
cpg	1098.19	J/molxK	1008.95	Joback Method
cpg	1111.46	J/molxK	1044.46	Joback Method
cpg	1123.10	J/molxK	1079.98	Joback Method
dvisc	0.0010437	Paxs	481.27	Joback Method
dvisc	0.0004977	Paxs	545.54	Joback Method

dvisc	0.0002774	Paxs	609.81	Joback Method
dvisc	0.0001729	Paxs	674.08	Joback Method
dvisc	0.0001170	Paxs	738.35	Joback Method
dvisc	0.0000842	Paxs	802.62	Joback Method
dvisc	0.0000637	Paxs	866.89	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=U339742&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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