

1,2-Cyclohexanedicarboxylic acid, allyl nonyl ester

Inchi:	InChI=1S/C20H34O4/c1-3-5-6-7-8-9-12-16-24-20(22)18-14-11-10-13-17(18)19(21)23-15
InchiKey:	RTQICOOOLQBUXRU-UHFFFAOYSA-N
Formula:	C20H34O4
SMILES:	C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCCC
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-245.74	kJ/mol	Joback Method
hf	-786.32	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	77.88	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.816		Crippen Method
mvol	292.380	ml/mol	McGowan Method
pc	1246.85	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	821.14	K	Joback Method
tc	1017.79	K	Joback Method
tf	460.86	K	Joback Method
vc	1.117	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.23	J/molxK	821.14	Joback Method
cpg	961.04	J/molxK	853.92	Joback Method
cpg	978.55	J/molxK	886.69	Joback Method
cpg	994.79	J/molxK	919.47	Joback Method
cpg	1009.77	J/molxK	952.24	Joback Method
cpg	1023.53	J/molxK	985.02	Joback Method
cpg	1036.07	J/molxK	1017.79	Joback Method
dvisc	0.0010265	Paxs	460.86	Joback Method

dvisc	0.0005171	Paxs	520.91	Joback Method
dvisc	0.0003001	Paxs	580.95	Joback Method
dvisc	0.0001929	Paxs	641.00	Joback Method
dvisc	0.0001337	Paxs	701.05	Joback Method
dvisc	0.0000982	Paxs	761.09	Joback Method
dvisc	0.0000755	Paxs	821.14	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=U339487&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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