

Dicyclohexyl suberate

Inchi:

InChI=1S/C20H34O4/c21-19(23-17-11-5-3-6-12-17)15-9-1-2-10-16-20(22)24-18-13-7-4-8

InchiKey:

VBSJUCDAWVFYNG-UHFFFAOYSA-N

Formula:

C20H34O4

SMILES:

O=C(CCCCCC(=O)OC1CCCCC1)OC1CCCCC1

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	-5.93		Crippen Method
logp	5.079		Crippen Method
mcvol	285.820	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2446.00		NIST Webbook
tb	848.68	K	Joback Method
tc	1062.77	K	Joback Method
tf	474.24	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.36	J/mol×K	848.68	Joback Method
cpg	983.22	J/mol×K	884.36	Joback Method
cpg	1001.42	J/mol×K	920.04	Joback Method
cpg	1017.99	J/mol×K	955.73	Joback Method
cpg	1032.97	J/mol×K	991.41	Joback Method
cpg	1046.37	J/mol×K	1027.09	Joback Method
cpg	1058.24	J/mol×K	1062.77	Joback Method
dvisc	0.0010931	Pa×s	474.24	Joback Method
dvisc	0.0005014	Pa×s	536.65	Joback Method

dvisc	0.0002705	Pa×s	599.05	Joback Method
dvisc	0.0001640	Pa×s	661.46	Joback Method
dvisc	0.0001083	Pa×s	723.87	Joback Method
dvisc	0.0000765	Pa×s	786.27	Joback Method
dvisc	0.0000568	Pa×s	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=R542500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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