

1,2-Cyclohexanedicarboxylic acid, allyl hexyl ester

Inchi:	InChI=1S/C17H28O4/c1-3-5-6-9-13-21-17(19)15-11-8-7-10-14(15)16(18)20-12-4-2/h4,14
InchiKey:	MWYODJPGJNHGMK-UHFFFAOYSA-N
Formula:	C17H28O4
SMILES:	C=CCOC(=O)C1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]:	296.40

Physical Properties

Property code	Value	Unit	Source
gf	-271.00	kJ/mol	Joback Method
hf	-724.40	kJ/mol	Joback Method
hfus	36.99	kJ/mol	Joback Method
hvap	71.20	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.645		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	752.50	K	Joback Method
tc	949.86	K	Joback Method
tf	427.05	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.03	J/molxK	752.50	Joback Method
cpg	844.69	J/molxK	916.97	Joback Method
cpg	830.85	J/molxK	884.07	Joback Method
cpg	815.89	J/molxK	851.18	Joback Method
cpg	799.77	J/molxK	818.29	Joback Method
cpg	782.49	J/molxK	785.39	Joback Method
cpg	857.39	J/molxK	949.86	Joback Method
dvisc	0.0001119	Paxs	752.50	Joback Method

dvisc	0.0001442	Paxs	698.26	Joback Method
dvisc	0.0001940	Paxs	644.02	Joback Method
dvisc	0.0002756	Paxs	589.77	Joback Method
dvisc	0.0004204	Paxs	535.53	Joback Method
dvisc	0.0007054	Paxs	481.29	Joback Method
dvisc	0.0013498	Paxs	427.05	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=U339484&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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