

1,2-Cyclohexanedicarboxylic acid, allyl butyl ester

Inchi:	InChI=1S/C15H24O4/c1-3-5-11-19-15(17)13-9-7-6-8-12(13)14(16)18-10-4-2/h4,12-13H,2
InchiKey:	AYLHMZJHXHVOOV-UHFFFAOYSA-N
Formula:	C15H24O4
SMILES:	C=CCOC(=O)C1CCCCC1C(=O)OCCCC
Mol. weight [g/mol]:	268.35

Physical Properties

Property code	Value	Unit	Source
gf	-287.84	kJ/mol	Joback Method
hf	-683.12	kJ/mol	Joback Method
hfus	31.81	kJ/mol	Joback Method
hvap	66.75	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.865		Crippen Method
mcvol	221.930	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinsol	1819.00		NIST Webbook
tb	706.74	K	Joback Method
tc	907.31	K	Joback Method
tf	404.51	K	Joback Method
vc	0.837	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.85	J/molxK	706.74	Joback Method
cpg	667.95	J/molxK	740.17	Joback Method
cpg	684.93	J/molxK	773.60	Joback Method
cpg	700.82	J/molxK	807.03	Joback Method
cpg	715.61	J/molxK	840.46	Joback Method
cpg	729.32	J/molxK	873.88	Joback Method
cpg	741.96	J/molxK	907.31	Joback Method
dvisc	0.0015743	Paxs	404.51	Joback Method
dvisc	0.0008455	Paxs	454.88	Joback Method

dvisc	0.0005140	Paxs	505.25	Joback Method
dvisc	0.0003420	Paxs	555.62	Joback Method
dvisc	0.0002435	Paxs	606.00	Joback Method
dvisc	0.0001826	Paxs	656.37	Joback Method
dvisc	0.0001427	Paxs	706.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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