

Cyclobutanecarboxylic acid, hexyl ester

Inchi:	InChI=1S/C11H20O2/c1-2-3-4-5-9-13-11(12)10-7-6-8-10/h10H,2-9H2,1H3
InchiKey:	RPGHXRQYDIQTCB-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CCCCCOC(=O)C1CCC1
Mol. weight [g/mol]:	184.28

Physical Properties

Property code	Value	Unit	Source
gf	-143.53	kJ/mol	Joback Method
hf	-448.53	kJ/mol	Joback Method
hfus	23.07	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.910		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinsol	1334.00		NIST Webbook
tb	538.38	K	Joback Method
tc	727.41	K	Joback Method
tf	300.31	K	Joback Method
vc	0.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.24	J/molxK	538.38	Joback Method
cpg	418.89	J/molxK	569.89	Joback Method
cpg	434.74	J/molxK	601.39	Joback Method
cpg	449.82	J/molxK	632.90	Joback Method
cpg	464.13	J/molxK	664.40	Joback Method
cpg	477.72	J/molxK	695.91	Joback Method
cpg	490.59	J/molxK	727.41	Joback Method
dvisc	0.0028040	Paxs	300.31	Joback Method
dvisc	0.0016198	Paxs	339.99	Joback Method

dvisc	0.0010495	Paxs	379.67	Joback Method
dvisc	0.0007381	Paxs	419.35	Joback Method
dvisc	0.0005517	Paxs	459.02	Joback Method
dvisc	0.0004320	Paxs	498.70	Joback Method
dvisc	0.0003506	Paxs	538.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U280403&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

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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