

Dihexyl oxalate

Inchi:	InChI=1S/C14H26O4/c1-3-5-7-9-11-17-13(15)14(16)18-12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey:	VIGLJKSIDLNMGH-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CCCCCOC(=O)C(=O)OCCCCC
Mol. weight [g/mol]:	258.35

Physical Properties

Property code	Value	Unit	Source
gf	-400.84	kJ/mol	Joback Method
hf	-821.89	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.233		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	672.30	K	Joback Method
tc	848.26	K	Joback Method
tf	391.86	K	Joback Method
vc	0.868	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.19	J/molxK	672.30	Joback Method
cpg	637.83	J/molxK	701.63	Joback Method
cpg	652.75	J/molxK	730.95	Joback Method
cpg	666.95	J/molxK	760.28	Joback Method
cpg	680.44	J/molxK	789.61	Joback Method
cpg	693.22	J/molxK	818.93	Joback Method

cpg	705.29	J/mol×K	848.26	Joback Method
dvisc	0.0014859	Paxs	391.86	Joback Method
dvisc	0.0007810	Paxs	438.60	Joback Method
dvisc	0.0004646	Paxs	485.34	Joback Method
dvisc	0.0003028	Paxs	532.08	Joback Method
dvisc	0.0002115	Paxs	578.82	Joback Method
dvisc	0.0001558	Paxs	625.56	Joback Method
dvisc	0.0001198	Paxs	672.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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