1,3-Dioxepane, 2-pentadecyl-

Inchi: InChI=1S/C20H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-21-18-15-16-19-22-20/h2
InchiKey: QZZVQKZZBUCTHK-UHFFFAOYSA-N
Formula: C20H40O2
SMILES: CCCCCCCCCCCCCCCC1OCCCCO1
Mol. weight [g/mol]: 312.53
CAS: 41563-29-5

Physical Properties

Property code	Value	Unit	Source
gf	-42.37	kJ/mol	Joback Method
hf	-671.97	kJ/mol	Joback Method
hfus	53.25	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.621		Crippen Method
mcvol	293.540	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
tb	734.72	K	Joback Method
tc	919.11	K	Joback Method
tf	372.16	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.51	J/mol×K	734.72	Joback Method
cpg	944.72	J/mol×K	765.45	Joback Method
cpg	965.73	J/mol×K	796.18	Joback Method
cpg	985.57	J/mol×K	826.91	Joback Method
cpg	1004.28	J/mol×K	857.65	Joback Method
cpg	1021.88	J/mol×K	888.38	Joback Method
cpg	1038.41	J/mol×K	919.11	Joback Method
dvisc	0.0030626	Pa×s	372.16	Joback Method
dvisc	0.0009989	Pa×s	432.59	Joback Method

dvisc	0.0004288	Pa×s	493.01	Joback Method
dvisc	0.0002214	Pa×s	553.44	Joback Method
dvisc	0.0001302	Pa×s	613.87	Joback Method
dvisc	0.0000842	Pa×s	674.29	Joback Method
dvisc	0.0000585	Pa×s	734.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41563295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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