Desmethyldoxepin

Other names: Nordoxepin
Inchi: InChI=1S/C18H19NO/c1-19-12-6-10-16-15-8-3-2-7-14(15)13-20-18-11-5-4-9-17(16)18/h2
InchiKey: HVKCEFHNSNZIHO-YBEGLDIGSA-N
Formula: C18H19NO
SMILES: CNCCC=C1c2ccccc2COc2ccccc21
Mol. weight [g/mol]: 265.35
CAS: 1225-56-5

Physical Properties

Property code	Value	Unit	Source
gf	423.43	kJ/mol	Joback Method
hf	125.91	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	73.49	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.620		Crippen Method
mcvol	217.650	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	2204.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	769.73	K	Joback Method
tc	1008.42	K	Joback Method
tf	482.27	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.43	J/mol×K	769.73	Joback Method
cpg	637.34	J/mol×K	809.51	Joback Method
cpg	652.13	J/mol×K	849.29	Joback Method
cpg	665.95	J/mol×K	889.07	Joback Method

cpg	678.91	J/mol×K	928.85	Joback Method
cpg	691.13	J/mol×K	968.63	Joback Method
cpg	702.76	J/mol×K	1008.42	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=C1225565&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
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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