1-Docosanol, formate

Other names: Docosanyl formate
Inchi: InChI=1S/C23H46O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-23
InchiKey: YOBPFSBRTYQJGQ-UHFFFAOYSA-N
Formula: C23H46O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCOC=O
Mol. weight [g/mol]: 354.61
CAS: 15155-62-1

Physical Properties

Property code	Value	Unit	Source
gf	-61.74	kJ/mol	Joback Method
hf	-735.85	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	75.92	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.981		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	881.04	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	796.72	K	Joback Method
tc	975.75	K	Joback Method
tf	413.20	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.86	J/mol×K	796.72	Joback Method
cpg	1112.91	J/mol×K	826.56	Joback Method
cpg	1132.90	J/mol×K	856.40	Joback Method
cpg	1151.85	J/mol×K	886.23	Joback Method
cpg	1169.80	J/mol×K	916.07	Joback Method
cpg	1186.78	J/mol×K	945.91	Joback Method

cpg	1202.83	J/mol×K	975.75	Joback Method
dvisc	0.0013966	Pa×s	413.20	Joback Method
dvisc	0.0005650	Pa×s	477.12	Joback Method
dvisc	0.0002831	Pa×s	541.04	Joback Method
dvisc	0.0001642	Pa×s	604.96	Joback Method
dvisc	0.0001056	Pa×s	668.88	Joback Method
dvisc	0.0000734	Pa×s	732.80	Joback Method
dvisc	0.0000541	Pa×s	796.72	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15155621&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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