

2-Docosanone

Inchi:	InChI=1S/C22H44O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(2)23/h3-
InchiKey:	TWBHLKOHVHGYGC-UHFFFAOYSA-N
Formula:	C22H44O
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]:	324.58
CAS:	77327-11-8

Physical Properties

Property code	Value	Unit	Source
gf	5.44	kJ/mol	Joback Method
hf	-609.99	kJ/mol	Joback Method
hfus	54.33	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	8.007		Crippen Method
mcvol	322.410	ml/mol	McGowan Method
pc	936.92	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	389.37		NIST Webbook
rinpol	389.37		NIST Webbook
tb	756.63	K	Joback Method
tc	930.05	K	Joback Method
tf	387.63	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.14	J/molxK	756.63	Joback Method
cpg	1017.85	J/molxK	785.53	Joback Method
cpg	1037.59	J/molxK	814.44	Joback Method
cpg	1056.38	J/molxK	843.34	Joback Method
cpg	1074.27	J/molxK	872.25	Joback Method
cpg	1091.28	J/molxK	901.15	Joback Method

cpg	1107.46	J/molxK	930.05	Joback Method
dvisc	0.0020125	Paxs	387.63	Joback Method
dvisc	0.0007953	Paxs	449.13	Joback Method
dvisc	0.0003931	Paxs	510.63	Joback Method
dvisc	0.0002260	Paxs	572.13	Joback Method
dvisc	0.0001447	Paxs	633.63	Joback Method
dvisc	0.0001003	Paxs	695.13	Joback Method
dvisc	0.0000737	Paxs	756.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48436e+01
Coeff. B	-5.50298e+03
Coeff. C	-1.22865e+02
Temperature range (K), min.	500.92
Temperature range (K), max.	700.17

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77327118&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor 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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