

isopentyl stearate

Inchi:	InChI=1S/C23H46O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(24)25-21-20-22
InchiKey:	WDQOEALRIMQDA-UHFFFAOYSA-N
Formula:	C23H46O2
SMILES:	CCCCCCCCCCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	354.61
CAS:	627-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-93.58	kJ/mol	Joback Method
hf	-768.13	kJ/mol	Joback Method
hfus	54.59	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	7.837		Crippen Method
mvol	342.370	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	2448.60		NIST Webbook
rinpol	2448.60		NIST Webbook
tb	801.49	K	Joback Method
tc	982.25	K	Joback Method
tf	406.13	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.96	J/molxK	801.49	Joback Method
cpg	1115.11	J/molxK	831.62	Joback Method
cpg	1135.16	J/molxK	861.74	Joback Method
cpg	1154.15	J/molxK	891.87	Joback Method
cpg	1172.09	J/molxK	921.99	Joback Method
cpg	1189.04	J/molxK	952.12	Joback Method
cpg	1205.01	J/molxK	982.25	Joback Method

dvisc	0.0014705	Paxs	406.13	Joback Method
dvisc	0.0005460	Paxs	472.02	Joback Method
dvisc	0.0002584	Paxs	537.92	Joback Method
dvisc	0.0001440	Paxs	603.81	Joback Method
dvisc	0.0000900	Paxs	669.70	Joback Method
dvisc	0.0000612	Paxs	735.60	Joback Method
dvisc	0.0000444	Paxs	801.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.05917e+01
Coeff. B	-8.32366e+03
Coeff. C	-1.39850e+02
Temperature range (K), min.	549.80
Temperature range (K), max.	684.58

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=C627883&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rincpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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