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: WDQOEAOLRIMQDA-UHFFFAOYSA-N
Formula: C23H46O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]: 354.62
CAS: 627-88-3

Physical Properties

Property code	Value	Unit	Source
af	1.0440		Cheméo Relay (1.0)
gf	-93.58	kJ/mol	Joback Method
hf	-841.99	kJ/mol	Cheméo Relay (1.0)
hfus	54.59	kJ/mol	Joback Method
hvap	106.68	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-7.74		Cheméo Relay (1.0)
logp	7.837		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	2448.60		NIST Webbook
rinpol	2448.60		NIST Webbook
tb	614.11	K	Cheméo Relay (1.0)
tc	792.80	K	Cheméo Relay (1.0)
tf	289.69	K	Cheméo Relay (1.0)
vc	1.334	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.96	J/mol×K	801.49	Joback Method
cpg	1205.01	J/mol×K	982.25	Joback Method
cpg	1189.04	J/mol×K	952.12	Joback Method
cpg	1172.09	J/mol×K	921.99	Joback Method
cpg	1154.15	J/mol×K	891.87	Joback Method

cpg	1135.16	J/mol×K	861.74	Joback Method
cpg	1115.11	J/mol×K	831.62	Joback Method
dvisc	0.0001440	Pa×s	603.81	Joback Method
dvisc	0.0000444	Pa×s	801.49	Joback Method
dvisc	0.0000612	Pa×s	735.60	Joback Method
dvisc	0.0000900	Pa×s	669.70	Joback Method
dvisc	0.0014705	Pa×s	406.13	Joback Method
dvisc	0.0002584	Pa×s	537.92	Joback Method
dvisc	0.0005460	Pa×s	472.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627883&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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