

Tangerinal 2

Inchi:	InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h8-9,12H,2-7,10-11H2,1H3
InchiKey:	MMCD SVCBSAMNPL-UHFFFAOYSA-N
Formula:	C12H22O
SMILES:	CCCCCCCC=CCCC=O
Mol. weight [g/mol]:	182.30

Physical Properties

Property code	Value	Unit	Source
gf	30.86	kJ/mol	Joback Method
hf	-259.37	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.882		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	526.78	K	Joback Method
tc	700.00	K	Joback Method
tf	261.92	K	Joback Method
vc	0.705	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.84	J/molxK	526.78	Joback Method
cpg	434.14	J/molxK	555.65	Joback Method
cpg	448.75	J/molxK	584.52	Joback Method
cpg	462.70	J/molxK	613.39	Joback Method
cpg	476.02	J/molxK	642.26	Joback Method
cpg	488.73	J/molxK	671.13	Joback Method
cpg	500.86	J/molxK	700.00	Joback Method

dvisc	0.0046993	Paxs	261.92	Joback Method
dvisc	0.0019373	Paxs	306.06	Joback Method
dvisc	0.0009985	Paxs	350.21	Joback Method
dvisc	0.0005970	Paxs	394.35	Joback Method
dvisc	0.0003959	Paxs	438.49	Joback Method
dvisc	0.0002830	Paxs	482.64	Joback Method
dvisc	0.0002140	Paxs	526.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410230&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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