

3-methylbutyl tetradecanoate

Other names:	isopentyl myristate Isopentyl tetradecanoate
Inchi:	InChI=1S/C19H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-19(20)21-17-16-18(2)3/h18H,4-1
InchiKey:	AISCBZKHUSXEOC-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	298.50
CAS:	62488-24-8

Physical Properties

Property code	Value	Unit	Source
gf	-127.26	kJ/mol	Joback Method
hf	-685.57	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	6.277		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2050.80		NIST Webbook
rinpol	2050.80		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2279.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2279.00		NIST Webbook
tb	709.97	K	Joback Method
tc	880.96	K	Joback Method
tf	361.05	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.12	J/mol×K	709.97	Joback Method

cpg	937.44	J/mol×K	852.46	Joback Method
cpg	921.48	J/mol×K	823.96	Joback Method
cpg	904.69	J/mol×K	795.46	Joback Method
cpg	887.04	J/mol×K	766.97	Joback Method
cpg	868.53	J/mol×K	738.47	Joback Method
cpg	952.60	J/mol×K	880.96	Joback Method
dvisc	0.0000774	Pa×s	709.97	Joback Method
dvisc	0.0001061	Pa×s	651.82	Joback Method
dvisc	0.0001546	Pa×s	593.66	Joback Method
dvisc	0.0002445	Pa×s	535.51	Joback Method
dvisc	0.0004323	Pa×s	477.36	Joback Method
dvisc	0.0008954	Pa×s	419.20	Joback Method
dvisc	0.0023450	Pa×s	361.05	Joback Method

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=C62488248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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