

Thymyl 2-methylbutyrate

Inchi:	InChI=1S/C15H22O2/c1-6-12(5)15(16)17-14-9-11(4)7-8-13(14)10(2)3/h7-10,12H,6H2,1-5
InchiKey:	NBUBCJBQVQEAAC-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCC(C)C(=O)Oc1cc(C)ccc1C(C)C
Mol. weight [g/mol]:	234.33
CAS:	69844-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-70.23	kJ/mol	Joback Method
hf	-394.70	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	60.96	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.070		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1571.10		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1571.10		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1964.00		NIST Webbook
tb	654.65	K	Joback Method
tc	861.20	K	Joback Method
tf	352.43	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.69	J/mol×K	654.65	Joback Method
cpg	563.79	J/mol×K	689.07	Joback Method
cpg	579.94	J/mol×K	723.50	Joback Method
cpg	595.15	J/mol×K	757.92	Joback Method
cpg	609.43	J/mol×K	792.35	Joback Method
cpg	622.82	J/mol×K	826.77	Joback Method
cpg	635.32	J/mol×K	861.20	Joback Method
dvisc	0.0018013	Paxs	352.43	Joback Method
dvisc	0.0008557	Paxs	402.80	Joback Method
dvisc	0.0004797	Paxs	453.17	Joback Method
dvisc	0.0003019	Paxs	503.54	Joback Method
dvisc	0.0002067	Paxs	553.91	Joback Method
dvisc	0.0001507	Paxs	604.28	Joback Method
dvisc	0.0001154	Paxs	654.65	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C69844322&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	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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