

2-Chloro-1-(2,4-dimethylphenyl)-2-methyl-1-propanone

Other names:	2-Chloro-1-(2,4-dimethylphenyl)-2-methyl-1-propanone
Inchi:	InChI=1S/C12H15ClO/c1-8-5-6-10(9(2)7-8)11(14)12(3,4)13/h5-7H,1-4H3
InchiKey:	FRXUQBIZUYXNKL-UHFFFAOYSA-N
Formula:	C12H15ClO
SMILES:	Cc1ccc(C(=O)C(C)(C)Cl)c(C)c1
Mol. weight [g/mol]:	210.70

Physical Properties

Property code	Value	Unit	Source
hf	-236.76	kJ/mol	Cheméo Relay (1.0)
hfus	18.48	kJ/mol	Joback Method
logp	3.504		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
tb	532.98	K	Cheméo Relay (1.0)
tf	312.10	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.09	J/mol×K	598.67	Joback Method
cpg	413.93	J/mol×K	636.56	Joback Method
cpg	427.74	J/mol×K	674.46	Joback Method
cpg	440.58	J/mol×K	712.35	Joback Method
cpg	452.51	J/mol×K	750.24	Joback Method
cpg	463.58	J/mol×K	788.14	Joback Method
cpg	473.87	J/mol×K	826.03	Joback Method
dvisc	0.0018407	Pa×s	358.73	Joback Method
dvisc	0.0010437	Pa×s	398.72	Joback Method
dvisc	0.0006563	Pa×s	438.71	Joback Method
dvisc	0.0004459	Pa×s	478.70	Joback Method
dvisc	0.0003216	Pa×s	518.69	Joback Method
dvisc	0.0002431	Pa×s	558.68	Joback Method
dvisc	0.0001907	Pa×s	598.67	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54965536&Units=SI>

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):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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