CUMINYL ACETATE

Other names:	Cuminyl acetate
	4-Isopropylbenzyl acetate
	Cuminic alcohol, acetate
	p-Cymen-7-ol acetate
	p-Isopropylbenzyl acetate
Inchi:	InChI=1S/C12H16O2/c1-9(2)12-6-4-11(5-7-12)8-14-10(3)13/h4-7,9H,8H2,1-3H3
InchiKey:	QBCRVYRADYXNOW-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(=O)OCc1ccc(C(C)C)cc1
Mol. weight [g/mol]:	192.26

Physical Properties

Property code	Value	Unit	Source
hf	-368.98	kJ/mol	Cheméo Relay (1.0)
hfus	19.75	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Cheméo Relay (1.0)
ie	8.45	eV	Cheméo Relay (1.0)
logp	2.873		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1401.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1952.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1981.00		NIST Webbook
tb	517.40	K	Cheméo Relay (1.0)
tc	727.74	K	Cheméo Relay (1.0)
tf	258.78	K	Cheméo Relay (1.0)
vc	0.596	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.16	J/mol×K	581.47	Joback Method
cpg	409.45	J/mol×K	616.69	Joback Method
cpg	423.89	J/mol×K	651.91	Joback Method
cpg	437.50	J/mol×K	687.12	Joback Method
cpg	450.30	J/mol×K	722.34	Joback Method
cpg	462.32	J/mol×K	757.56	Joback Method
cpg	473.55	J/mol×K	792.78	Joback Method
dvisc	0.0021607	Pa×s	321.10	Joback Method
dvisc	0.0010969	Pa×s	364.50	Joback Method
dvisc	0.0006432	Pa×s	407.89	Joback Method
dvisc	0.0004180	Pa×s	451.29	Joback Method
dvisc	0.0002929	Pa×s	494.68	Joback Method
dvisc	0.0002174	Pa×s	538.08	Joback Method
dvisc	0.0001687	Pa×s	581.47	Joback Method

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59230578&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy

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