6-METHYL COUMARIN

Other names:	Coumarin, 6-methyl- Toncarine 6-Methylbenzopyrone 6-Methylcoumarin 6-Methylcoumarinic anhydride 6-MC 6-Methylcumarin NCI-C55812 6-Methyl-1,2-benzopyrone 6-Methyl-2H-1-benzopyran-2-one NSC 5870
Inchi:	InChI=1S/C10H8O2/c1-7-2-4-9-8(6-7)3-5-10(11)12-9/h2-6H,1H3
InchiKey:	FXFYOPQLGGEACP-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	Cc1ccc2oc(=O)ccc2c1
Mol. weight [g/mol]:	160.17

Physical Properties

Property code	Value	Unit	Source
af	0.4929		Cheméo Relay (1.0)
gf	-84.05	kJ/mol	Cheméo Relay (1.0, beta)
hf	-202.83	kJ/mol	Cheméo Relay (1.0)
hvap	85.60	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-2.66		Cheméo Relay (1.0)
logp	2.101		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
pc	3939.22	kPa	Cheméo Relay (1.0, beta)
rinpol	1574.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1545.00		NIST Webbook
ripol	2560.00		NIST Webbook
ripol	2551.00		NIST Webbook

ripol	2630.00		NIST Webbook
ripol	2630.00		NIST Webbook
ripol	2551.00		NIST Webbook
tb	580.83	K	Cheméo Relay (1.0)
tc	790.36	K	Cheméo Relay (1.0)
tf	357.76	K	Cheméo Relay (1.0)
vc	0.454	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	576.20	K	96.70	NIST Webbook
tbrp	447.20	K	1.90	NIST Webbook

Sources

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=C92488&Units=SI

Legend

af: Acentric Factor
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume