DIMETHYL 5,6-ACENAPHTHENEDICARBOXYLATE

Other names: 5,6-Dicarbomethoxyacenaphthene
Inchi: InChI=1S/C16H14O4/c1-19-15(17)11-7-5-9-3-4-10-6-8-12(16(18)20-2)14(11)13(9)10/h5-
InchiKey: KZDDQWFGWDKABI-UHFFFAOYSA-N
Formula: C16H14O4
SMILES: COC(=O)c1ccc2c3c(ccc(C(=O)OC)c13)CC2
Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
hf	-528.62	kJ/mol	Cheméo Relay (1.0)
hfus	31.44	kJ/mol	Joback Method
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-4.47		Cheméo Relay (1.0)
logp	2.512		Crippen Method
mcvol	197.100	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	654.83	K	Cheméo Relay (1.0)
tc	922.75	K	Cheméo Relay (1.0)
tf	428.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.52	J/mol×K	982.83	Joback Method
cpg	614.63	J/mol×K	1021.25	Joback Method
cpg	563.27	J/mol×K	829.19	Joback Method
cpg	574.85	J/mol×K	867.60	Joback Method
cpg	585.71	J/mol×K	906.01	Joback Method
cpg	595.91	J/mol×K	944.42	Joback Method
cpg	550.89	J/mol×K	790.78	Joback Method
dvisc	0.0010083	Pa×s	629.79	Joback Method
dvisc	0.0011996	Pa×s	589.55	Joback Method
dvisc	0.0014641	Pa×s	549.30	Joback Method
dvisc	0.0008654	Pa×s	670.04	Joback Method

dvisc	0.0007557	Pa×s	710.29	Joback Method
dvisc	0.0006696	Pa×s	750.53	Joback Method
dvisc	0.0006006	Pa×s	790.78	Joback Method
hfust	34.73	kJ/mol	450.20	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4599966&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
hfust: Enthalpy of fusion at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point