METHYL HYDROGEN SEBACATE

Other names:	Mono-methyl sebacate
	Decanedioic acid, monomethyl ester
	Methyl hydrogen sebacate
Inchi:	InChI=1S/C11H20O4/c1-15-11(14)9-7-5-3-2-4-6-8-10(12)13/h2-9H2,1H3,(H,12,13)
InchiKey:	OSYQOBUUFRGFNG-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	COC(=O)CCCCCCCCC(=O)O
Mol. weight [g/mol]:	216.28

Physical Properties

Property code	Value	Unit	Source
af	0.9123		Cheméo Relay (1.0)
gf	-457.92	kJ/mol	Joback Method
hf	-908.48	kJ/mol	Cheméo Relay (1.0)
hfus	32.72	kJ/mol	Joback Method
hvap	106.17	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-2.52		Cheméo Relay (1.0)
logp	2.365		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
tb	567.05	K	Cheméo Relay (1.0)
tc	750.73	K	Cheméo Relay (1.0)
tf	315.90 ± 1.00	K	NIST Webbook
vc	0.687	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.54	J/mol×K	673.42	Joback Method
cpg	509.64	J/mol×K	702.50	Joback Method
cpg	521.16	J/mol×K	731.58	Joback Method

cpg	532.12	J/mol×K	760.66	Joback Method
cpg	542.52	J/mol×K	789.74	Joback Method
cpg	552.38	J/mol×K	818.82	Joback Method
cpg	561.70	J/mol×K	847.91	Joback Method
dvisc	0.0024766	Pa×s	396.64	Joback Method
dvisc	0.0009420	Pa×s	442.77	Joback Method
dvisc	0.0004300	Pa×s	488.90	Joback Method
dvisc	0.0002247	Pa×s	535.03	Joback Method
dvisc	0.0001301	Pa×s	581.16	Joback Method
dvisc	0.0000817	Pa×s	627.29	Joback Method
dvisc	0.0000547	Pa×s	673.42	Joback Method

Sources

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=C818882&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

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

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

tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume