Sebacic acid monomethyl ester

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]:	216.27
CAS:	818-88-2

Physical Properties

Property code	Value	Unit	Source
gf	-457.92	kJ/mol	Joback Method
hf	-779.98	kJ/mol	Joback Method
hfus	32.72	kJ/mol	Joback Method
hvap	72.66	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
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	673.42	K	Joback Method
tc	847.91	K	Joback Method
tf	315.90 ± 1.00	K	NIST Webbook
vc	0.701	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C818882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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

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