Ethyl hydrogen fumarate

Other names:	Monoethyl fumarate
	Fumaric acid monoethyl ester
	2-Butenedioic acid (E)-, monoethyl ester
	ethyl fumarate
Inchi:	InChI=1S/C6H8O4/c1-2-10-6(9)4-3-5(7)8/h3-4H,2H2,1H3,(H,7,8)/b4-3+
InchiKey:	XLYMOEINVGRTEX-ONEGZZNKSA-N
Formula:	C6H8O4
SMILES:	CCOC(=O)C=CC(=O)O
Mol. weight [g/mol]:	144.13
CAS:	2459-05-4

Physical Properties

Property code	Value	Unit	Source
gf	-419.80	kJ/mol	Joback Method
hf	-559.56	kJ/mol	Joback Method
hfus	19.97	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	0.190		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	563.18	K	Joback Method
tc	750.05	K	Joback Method
tf	335.21	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.03	J/mol×K	563.18	Joback Method
cpg	245.59	J/mol×K	594.32	Joback Method
cpg	252.78	J/mol×K	625.47	Joback Method
cpg	259.61	J/mol×K	656.61	Joback Method
cpg	266.10	J/mol×K	687.76	Joback Method

cpg	272.24	J/mol×K	718.90	Joback Method
cpg	278.04	J/mol×K	750.05	Joback Method
dvisc	0.0051297	Pa×s	335.21	Joback Method
dvisc	0.0019494	Pa×s	373.21	Joback Method
dvisc	0.0008858	Pa×s	411.20	Joback Method
dvisc	0.0004600	Pa×s	449.20	Joback Method
dvisc	0.0002646	Pa×s	487.19	Joback Method
dvisc	0.0001649	Pa×s	525.19	Joback Method
dvisc	0.0001095	Pa×s	563.18	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.20	K	2.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2459054&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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume