1,2-Benzenedicarboxylic acid, ethyl methyl ester

Other names: Ethyl methyl phthalate
Inchi: InChI=1S/C11H12O4/c1-3-15-11(13)9-7-5-4-6-8(9)10(12)14-2/h4-7H,3H2,1-2H3
InchiKey: HGERXYZHJFOFNE-UHFFFAOYSA-N
Formula: C11H12O4
SMILES: CCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]: 208.21
CAS: 34006-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-323.32	kJ/mol	Joback Method
hf	-534.91	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.650		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1499.00		NIST Webbook
ripol	2315.00		NIST Webbook
tb	635.32	K	Joback Method
tc	850.61	K	Joback Method
tf	396.99	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.89	J/mol×K	635.32	Joback Method
cpg	442.73	J/mol×K	814.73	Joback Method
cpg	433.09	J/mol×K	778.85	Joback Method
cpg	422.68	J/mol×K	742.97	Joback Method
cpg	411.51	J/mol×K	707.08	Joback Method
cpg	399.58	J/mol×K	671.20	Joback Method

cpg	451.61	J/mol×K	850.61	Joback Method
dvisc	0.0001656	Pa×s	635.32	Joback Method
dvisc	0.0002056	Pa×s	595.60	Joback Method
dvisc	0.0002634	Pa×s	555.88	Joback Method
dvisc	0.0003506	Pa×s	516.15	Joback Method
dvisc	0.0004894	Pa×s	476.43	Joback Method
dvisc	0.0007259	Pa×s	436.71	Joback Method
dvisc	0.0011650	Pa×s	396.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34006774&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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