

(R)-(+)-3-Methyladipic acid

Other names:	(+)-3-Methyladipic acid Hexanedioic acid, 3-methyl-, (R)-
Inchi:	InChI=1S/C7H12O4/c1-5(4-7(10)11)2-3-6(8)9/h5H,2-4H2,1H3,(H,8,9)(H,10,11)
InchiKey:	SYEOWUNSTUDKGM-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CC(CCC(=O)O)CC(=O)O
Mol. weight [g/mol]:	160.17
CAS:	623-82-5

Physical Properties

Property code	Value	Unit	Source
gf	-525.86	kJ/mol	Joback Method
hf	-722.71	kJ/mol	Joback Method
hfus	21.74	kJ/mol	Joback Method
h vap	77.64	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.962		Crippen Method
m cvol	124.370	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	651.22	K	Joback Method
tc	826.91	K	Joback Method
tf	375.15	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.86	J/mol×K	651.22	Joback Method
cpg	360.95	J/mol×K	797.63	Joback Method
cpg	354.49	J/mol×K	768.35	Joback Method
cpg	347.66	J/mol×K	739.07	Joback Method
cpg	340.46	J/mol×K	709.78	Joback Method
cpg	332.86	J/mol×K	680.50	Joback Method
cpg	367.05	J/mol×K	826.91	Joback Method

dvisc	0.0000280	Paxs	651.22	Joback Method
dvisc	0.0000498	Paxs	605.21	Joback Method
dvisc	0.0000974	Paxs	559.20	Joback Method
dvisc	0.0002150	Paxs	513.19	Joback Method
dvisc	0.0005549	Paxs	467.17	Joback Method
dvisc	0.0017611	Paxs	421.16	Joback Method
dvisc	0.0074203	Paxs	375.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	503.20	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.77303e+01
Coeff. B	-6.45093e+03
Coeff. C	-1.09965e+02
Temperature range (K), min.	479.80
Temperature range (K), max.	629.41

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623825&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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