

Adipic acid, butyl pent-4-en-2-yl ester

Inchi:	InChI=1S/C15H26O4/c1-4-6-12-18-14(16)10-7-8-11-15(17)19-13(3)9-5-2/h5,13H,2,4,6-1
InchiKey:	FORLKMRJCQLQRG-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	C=CCC(C)OC(=O)CCCC(=O)OCCCC
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-307.02	kJ/mol	Joback Method
hf	-722.38	kJ/mol	Joback Method
hfus	35.38	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.398		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinsol	1769.00		NIST Webbook
tb	691.42	K	Joback Method
tc	871.43	K	Joback Method
tf	386.37	K	Joback Method
vc	0.898	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.86	J/molxK	691.42	Joback Method
cpg	669.68	J/molxK	721.42	Joback Method
cpg	684.71	J/molxK	751.42	Joback Method
cpg	698.97	J/molxK	781.43	Joback Method
cpg	712.46	J/molxK	811.43	Joback Method
cpg	725.19	J/molxK	841.43	Joback Method
cpg	737.18	J/molxK	871.43	Joback Method
dvisc	0.0016556	Paxs	386.37	Joback Method
dvisc	0.0007963	Paxs	437.21	Joback Method

dvisc	0.0004461	Paxs	488.05	Joback Method
dvisc	0.0002788	Paxs	538.89	Joback Method
dvisc	0.0001889	Paxs	589.74	Joback Method
dvisc	0.0001362	Paxs	640.58	Joback Method
dvisc	0.0001030	Paxs	691.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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