

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

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

Physical Properties

Property code	Value	Unit	Source
gf	-309.46	kJ/mol	Joback Method
hf	-727.66	kJ/mol	Joback Method
hfus	31.85	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.254		Crippen Method
mvol	232.790	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		NIST Webbook
tb	690.98	K	Joback Method
tc	873.40	K	Joback Method
tf	371.37	K	Joback Method
vc	0.892	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.33	J/molxK	690.98	Joback Method
cpg	670.39	J/molxK	721.38	Joback Method
cpg	685.64	J/molxK	751.79	Joback Method
cpg	700.07	J/molxK	782.19	Joback Method
cpg	713.72	J/molxK	812.59	Joback Method
cpg	726.57	J/molxK	842.99	Joback Method
cpg	738.65	J/molxK	873.40	Joback Method
dvisc	0.0020674	Paxs	371.37	Joback Method

dvisc	0.0008976	Paxs	424.64	Joback Method
dvisc	0.0004694	Paxs	477.91	Joback Method
dvisc	0.0002795	Paxs	531.17	Joback Method
dvisc	0.0001830	Paxs	584.44	Joback Method
dvisc	0.0001286	Paxs	637.71	Joback Method
dvisc	0.0000954	Paxs	690.98	Joback Method

Sources

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=U354118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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