

Adipic acid, 2,3-dimethylphenyl isobutyl ester

Inchi:	InChI=1S/C18H26O4/c1-13(2)12-21-17(19)10-5-6-11-18(20)22-16-9-7-8-14(3)15(16)4/h
InchiKey:	WLAAZWPBTZUWOS-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	<chem>Cc1cccc(OC(=O)CCCCC(=O)OCC(C)C)c1C</chem>
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-276.45	kJ/mol	Joback Method
hf	-696.14	kJ/mol	Joback Method
hfus	37.69	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.968		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2236.00		NIST Webbook
tb	800.02	K	Joback Method
tc	1002.86	K	Joback Method
tf	473.40	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.07	J/molxK	800.02	Joback Method
cpg	776.84	J/molxK	833.83	Joback Method
cpg	791.53	J/molxK	867.63	Joback Method
cpg	805.16	J/molxK	901.44	Joback Method
cpg	817.74	J/molxK	935.25	Joback Method
cpg	829.27	J/molxK	969.06	Joback Method
cpg	839.79	J/molxK	1002.86	Joback Method
dvisc	0.0006911	Paxs	473.40	Joback Method
dvisc	0.0003829	Paxs	527.84	Joback Method

dvisc	0.0002369	Paxs	582.27	Joback Method
dvisc	0.0001591	Paxs	636.71	Joback Method
dvisc	0.0001138	Paxs	691.15	Joback Method
dvisc	0.0000855	Paxs	745.58	Joback Method
dvisc	0.0000667	Paxs	800.02	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=U353880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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