

Adipic acid, butyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C18H26O4/c1-4-5-13-21-17(19)11-6-7-12-18(20)22-16-10-8-9-14(2)15(16)3/h8-17
InchiKey: OODL UFCFTUJGAK-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCOC(=O)CCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-274.01	kJ/mol	Joback Method
hf	-690.86	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	77.57	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.113		Crippen Method
mvol	255.600	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	2280.00		NIST Webbook
tb	800.46	K	Joback Method
tc	1000.95	K	Joback Method
tf	488.40	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.53	J/molxK	800.46	Joback Method
cpg	776.12	J/molxK	833.88	Joback Method
cpg	790.66	J/molxK	867.29	Joback Method
cpg	804.18	J/molxK	900.71	Joback Method
cpg	816.68	J/molxK	934.12	Joback Method
cpg	828.18	J/molxK	967.54	Joback Method
cpg	838.68	J/molxK	1000.95	Joback Method
dvisc	0.0006133	Paxs	488.40	Joback Method
dvisc	0.0003622	Paxs	540.41	Joback Method

dvisc	0.0002346	Paxs	592.42	Joback Method
dvisc	0.0001630	Paxs	644.43	Joback Method
dvisc	0.0001196	Paxs	696.44	Joback Method
dvisc	0.0000916	Paxs	748.45	Joback Method
dvisc	0.0000726	Paxs	800.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353881&Units=SI

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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