

Adipic acid, butyl 2,4-dimethylpent-3-yl ester

Inchi:	InChI=1S/C17H32O4/c1-6-7-12-20-15(18)10-8-9-11-16(19)21-17(13(2)3)14(4)5/h13-14,1
InchiKey:	XSCNOJMTCNMZEE-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCOC(=O)CCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-382.90	kJ/mol	Joback Method
hf	-899.65	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.114		Crippen Method
mvol	265.270	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook
tb	739.62	K	Joback Method
tc	922.00	K	Joback Method
tf	380.67	K	Joback Method
vc	1.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.48	J/molxK	739.62	Joback Method
cpg	810.02	J/molxK	770.02	Joback Method
cpg	826.62	J/molxK	800.41	Joback Method
cpg	842.29	J/molxK	830.81	Joback Method
cpg	857.04	J/molxK	861.21	Joback Method
cpg	870.89	J/molxK	891.60	Joback Method
cpg	883.84	J/molxK	922.00	Joback Method
dvisc	0.0021500	Paxs	380.67	Joback Method

dvisc	0.0008028	Paxs	440.50	Joback Method
dvisc	0.0003794	Paxs	500.32	Joback Method
dvisc	0.0002104	Paxs	560.14	Joback Method
dvisc	0.0001308	Paxs	619.97	Joback Method
dvisc	0.0000884	Paxs	679.80	Joback Method
dvisc	0.0000636	Paxs	739.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349777&Units=SI
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
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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