

Adipic acid, butyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C12H19Cl3O4/c1-2-3-8-18-10(16)6-4-5-7-11(17)19-9-12(13,14)15/h2-9H2,1H3
InchiKey:	JTPBVPBJYDQUIX-UHFFFAOYSA-N
Formula:	C12H19Cl3O4
SMILES:	CCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	333.64

Physical Properties

Property code	Value	Unit	Source
gf	-450.63	kJ/mol	Joback Method
hf	-836.58	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.803		Crippen Method
mcvol	231.540	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpola	1963.00		NIST Webbook
rinpola	1963.00		NIST Webbook
tb	735.60	K	Joback Method
tc	933.37	K	Joback Method
tf	461.50	K	Joback Method
vc	0.891	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.52	J/molxK	735.60	Joback Method
cpg	613.90	J/molxK	768.56	Joback Method
cpg	625.49	J/molxK	801.52	Joback Method
cpg	636.31	J/molxK	834.49	Joback Method
cpg	646.38	J/molxK	867.45	Joback Method
cpg	655.72	J/molxK	900.41	Joback Method
cpg	664.35	J/molxK	933.37	Joback Method
dvisc	0.0009510	Paxs	461.50	Joback Method

dvisc	0.0005367	Paxs	507.18	Joback Method
dvisc	0.0003329	Paxs	552.87	Joback Method
dvisc	0.0002221	Paxs	598.55	Joback Method
dvisc	0.0001569	Paxs	644.23	Joback Method
dvisc	0.0001161	Paxs	689.92	Joback Method
dvisc	0.0000892	Paxs	735.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353476&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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