

Adipic acid, 2,2-dichloroethyl isobutyl ester

Inchi:	InChI=1S/C12H20Cl2O4/c1-9(2)7-17-11(15)5-3-4-6-12(16)18-8-10(13)14/h9-10H,3-8H2,
InchiKey:	CPCFIRJBGFNZLS-UHFFFAOYSA-N
Formula:	C12H20Cl2O4
SMILES:	CC(C)COC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	299.19

Physical Properties

Property code	Value	Unit	Source
gf	-446.42	kJ/mol	Joback Method
hf	-822.65	kJ/mol	Joback Method
hfus	33.76	kJ/mol	Joback Method
hvap	68.61	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.093		Crippen Method
mvol	219.300	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1852.00		NIST Webbook
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tb	700.52	K	Joback Method
tc	892.04	K	Joback Method
tf	399.16	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.07	J/molxK	700.52	Joback Method
cpg	633.88	J/molxK	860.12	Joback Method
cpg	623.41	J/molxK	828.20	Joback Method
cpg	612.20	J/molxK	796.28	Joback Method
cpg	600.25	J/molxK	764.36	Joback Method
cpg	587.54	J/molxK	732.44	Joback Method
cpg	643.60	J/molxK	892.04	Joback Method
dvisc	0.0001058	Paxs	700.52	Joback Method

dvisc	0.0001408	Paxs	650.29	Joback Method
dvisc	0.0001967	Paxs	600.07	Joback Method
dvisc	0.0002919	Paxs	549.84	Joback Method
dvisc	0.0004692	Paxs	499.61	Joback Method
dvisc	0.0008385	Paxs	449.39	Joback Method
dvisc	0.0017341	Paxs	399.16	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=U353577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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