

Sebacic acid, butyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C16H28Cl2O4/c1-2-3-12-21-15(19)10-8-6-4-5-7-9-11-16(20)22-13-14(17)18/h
InchiKey:	PYAHDMOPOYFLQI-UHFFFAOYSA-N
Formula:	C16H28Cl2O4
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	355.30

Physical Properties

Property code	Value	Unit	Source
gf	-410.30	kJ/mol	Joback Method
hf	-899.93	kJ/mol	Joback Method
hfus	47.64	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.797		Crippen Method
mvol	275.660	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2337.00		NIST Webbook
rinpol	2337.00		NIST Webbook
tb	792.48	K	Joback Method
tc	980.97	K	Joback Method
tf	459.24	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.61	J/molxK	792.48	Joback Method
cpg	809.56	J/molxK	823.89	Joback Method
cpg	823.60	J/molxK	855.31	Joback Method
cpg	836.74	J/molxK	886.72	Joback Method
cpg	849.01	J/molxK	918.14	Joback Method
cpg	860.40	J/molxK	949.55	Joback Method
cpg	870.93	J/molxK	980.97	Joback Method
dvisc	0.0009489	Paxs	459.24	Joback Method

dvisc	0.0004763	Paxs	514.78	Joback Method
dvisc	0.0002734	Paxs	570.32	Joback Method
dvisc	0.0001732	Paxs	625.86	Joback Method
dvisc	0.0001182	Paxs	681.40	Joback Method
dvisc	0.0000854	Paxs	736.94	Joback Method
dvisc	0.0000646	Paxs	792.48	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=U355468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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