

Sebacic acid, di(2,4,6-trichlorobenzyl) ester

Inchi: InChI=1S/C24H24Cl6O4/c25-15-9-19(27)17(20(28)10-15)13-33-23(31)7-5-3-1-2-4-6-8-24
InchiKey: NISMECQHDIIBEJ-UHFFFAOYSA-N
Formula: C24H24Cl6O4
SMILES: O=C(CCCCCCCCC(=O)OCc1c(Cl)cc(Cl)cc1Cl)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 589.16

Physical Properties

Property code	Value	Unit	Source
gf	-221.18	kJ/mol	Joback Method
hf	-718.49	kJ/mol	Joback Method
hfus	74.42	kJ/mol	Joback Method
hvap	122.16	kJ/mol	Joback Method
log10ws	-10.90		Crippen Method
logp	9.514		Crippen Method
mcvol	389.820	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	3687.00		NIST Webbook
tb	1208.92	K	Joback Method
tc	1481.31	K	Joback Method
tf	812.04	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1113.86	J/molxK	1208.92	Joback Method
cpg	1122.15	J/molxK	1435.91	Joback Method
cpg	1123.73	J/molxK	1390.51	Joback Method
cpg	1123.74	J/molxK	1345.12	Joback Method
cpg	1122.14	J/molxK	1299.72	Joback Method
cpg	1118.86	J/molxK	1254.32	Joback Method
cpg	1119.08	J/molxK	1481.31	Joback Method
dvisc	0.0000124	Paxs	1208.92	Joback Method
dvisc	0.0000151	Paxs	1142.77	Joback Method

dvisc	0.0000189	Paxs	1076.63	Joback Method
dvisc	0.0000242	Paxs	1010.48	Joback Method
dvisc	0.0000321	Paxs	944.33	Joback Method
dvisc	0.0000445	Paxs	878.19	Joback Method
dvisc	0.0000651	Paxs	812.04	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=U380578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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