

Sebacic acid, di(2,5-dichlorobenzyl) ester

Inchi: InChI=1S/C24H26Cl4O4/c25-19-9-11-21(27)17(13-19)15-31-23(29)7-5-3-1-2-4-6-8-24(30)
InchiKey: IBXJOIYFXHXUTH-UHFFFAOYSA-N
Formula: C24H26Cl4O4
SMILES: O=C(CCCCCCCC(=O)OCc1cc(Cl)ccc1Cl)OCc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 520.27

Physical Properties

Property code	Value	Unit	Source
gf	-178.06	kJ/mol	Joback Method
hf	-664.07	kJ/mol	Joback Method
hfus	66.80	kJ/mol	Joback Method
hvap	112.07	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.208		Crippen Method
mcvol	365.340	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	3566.00		NIST Webbook
rinpol	3566.00		NIST Webbook
tb	1124.10	K	Joback Method
tc	1376.29	K	Joback Method
tf	727.16	K	Joback Method
vc	1.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.07	J/molxK	1124.10	Joback Method
cpg	1119.23	J/molxK	1334.26	Joback Method
cpg	1116.39	J/molxK	1292.23	Joback Method
cpg	1112.22	J/molxK	1250.20	Joback Method
cpg	1106.64	J/molxK	1208.16	Joback Method
cpg	1099.61	J/molxK	1166.13	Joback Method
cpg	1120.79	J/molxK	1376.29	Joback Method
dvisc	0.0000171	Paxs	1124.10	Joback Method

dvisc	0.0000212	Paxs	1057.94	Joback Method
dvisc	0.0000270	Paxs	991.79	Joback Method
dvisc	0.0000356	Paxs	925.63	Joback Method
dvisc	0.0000491	Paxs	859.47	Joback Method
dvisc	0.0000714	Paxs	793.32	Joback Method
dvisc	0.0001110	Paxs	727.16	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=U380621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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