Sebacic acid, 2,4-dichlorophenyl isobutyl ester

Inchi: InChI=1S/C20H28Cl2O4/c1-15(2)14-25-19(23)9-7-5-3-4-6-8-10-20(24)26-18-12-11-16(21

InchiKey: PJAZYWNLDWQLSI-UHFFFAOYSA-N

Formula: C20H28Cl2O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 403.34

Physical Properties

Property code	Value	Unit	Source
gf	-283.47	kJ/mol	Joback Method
hf	-768.90	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.219		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook
tb	920.64	K	Joback Method
tc	1133.87	K	Joback Method
tf	555.78	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.62	J/mol×K	920.64	Joback Method
cpg	943.37	J/mol×K	956.18	Joback Method
cpg	955.91	J/mol×K	991.72	Joback Method
cpg	967.26	J/mol×K	1027.25	Joback Method
cpg	977.44	J/mol×K	1062.79	Joback Method
cpg	986.48	J/mol×K	1098.33	Joback Method
cpg	994.41	J/mol×K	1133.87	Joback Method
dvisc	0.0003776	Pa×s	555.78	Joback Method

dvisc	0.0002124	Pa×s	616.59	Joback Method
dvisc	0.0001325	Pa×s	677.40	Joback Method
dvisc	0.0000893	Pa×s	738.21	Joback Method
dvisc	0.0000640	Pa×s	799.02	Joback Method
dvisc	0.0000480	Pa×s	859.83	Joback Method
dvisc	0.0000374	Pa×s	920.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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