

Sebacic acid, butyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C20H27Cl3O4/c1-2-3-12-26-18(24)10-8-6-4-5-7-9-11-19(25)27-20-16(22)13-15
InchiKey: MNNNNRBLUWYTQ-UHFFFAOYSA-N
Formula: C20H27Cl3O4
SMILES: CCCCOC(=O)CCCCCCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 437.79

Physical Properties

Property code	Value	Unit	Source
gf	-302.59	kJ/mol	Joback Method
hf	-790.83	kJ/mol	Joback Method
hfus	58.59	kJ/mol	Joback Method
hvap	95.84	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	7.016		Crippen Method
mvol	320.500	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook
tb	963.49	K	Joback Method
tc	1182.62	K	Joback Method
tf	613.22	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.93	J/molxK	963.49	Joback Method
cpg	963.35	J/molxK	1000.01	Joback Method
cpg	974.53	J/molxK	1036.53	Joback Method
cpg	984.50	J/molxK	1073.05	Joback Method
cpg	993.26	J/molxK	1109.58	Joback Method
cpg	1000.85	J/molxK	1146.10	Joback Method
cpg	1007.29	J/molxK	1182.62	Joback Method
dvisc	0.0002540	Paxs	613.22	Joback Method

dvisc	0.0001586	Paxs	671.60	Joback Method
dvisc	0.0001068	Paxs	729.98	Joback Method
dvisc	0.0000762	Paxs	788.36	Joback Method
dvisc	0.0000570	Paxs	846.73	Joback Method
dvisc	0.0000442	Paxs	905.11	Joback Method
dvisc	0.0000354	Paxs	963.49	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=U355077&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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