DIBENZYL ADIPATE

Other names: dibenzyl adipate
Inchi: InChI=1S/C20H22O4/c21-19(23-15-17-9-3-1-4-10-17)13-7-8-14-20(22)24-16-18-11-5-2-6
InchiKey: AEUORZZHALJMBM-UHFFFAOYSA-N
Formula: C20H22O4
SMILES: O=C(CCCCC(=O)OCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
hfus	41.21	kJ/mol	Joback Method
hvap	109.20	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-4.29		Cheméo Relay (1.0)
logp	4.034		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	2616.00		NIST Webbook
tb	652.59	K	Cheméo Relay (1.0)
tc	894.10	K	Cheméo Relay (1.0)
tf	311.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.60	J/mol×K	862.94	Joback Method
cpg	796.90	J/mol×K	900.11	Joback Method
cpg	809.92	J/mol×K	937.28	Joback Method
cpg	821.72	J/mol×K	974.45	Joback Method
cpg	832.33	J/mol×K	1011.62	Joback Method
cpg	841.80	J/mol×K	1048.79	Joback Method
cpg	850.18	J/mol×K	1085.96	Joback Method
dvisc	0.0005956	Pa×s	512.32	Joback Method
dvisc	0.0003272	Pa×s	570.76	Joback Method
dvisc	0.0002009	Pa×s	629.19	Joback Method

dvisc	0.0001340	Pa×s	687.63	Joback Method
dvisc	0.0000953	Pa×s	746.07	Joback Method
dvisc	0.0000712	Pa×s	804.50	Joback Method
dvisc	0.0000553	Pa×s	862.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2451845&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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