

1,4-benzenedicarboxylic acid, diheptyl ester

Other names:	1,4-Benzenedicarboxylic acid, diheptyl ester
Inchi:	InChI=1S/C22H34O4/c1-3-5-7-9-11-17-25-21(23)19-13-15-20(16-14-19)22(24)26-18-12-
InchiKey:	RXDQUKGEPHJIJN-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCCCCOC(=O)c1ccc(C(=O)OCCCCCCC)cc1
Mol. weight [g/mol]:	362.50
CAS:	4654-25-5

Physical Properties

Property code	Value	Unit	Source
af	1.0978		Cheméo Relay (1.0)
hf	-880.73	kJ/mol	Cheméo Relay (1.0)
hfus	51.96	kJ/mol	Joback Method
hvap	107.87	kJ/mol	Cheméo Relay (1.0)
ie	9.35	eV	Cheméo Relay (1.0)
log10ws	-6.59		Cheméo Relay (1.0)
logp	5.941		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
tb	650.80	K	Cheméo Relay (1.0)
tc	844.38	K	Cheméo Relay (1.0)
tf	312.64	K	Cheméo Relay (1.0)
vc	1.188	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.29	J/mol×K	887.00	Joback Method
cpg	1013.85	J/mol×K	920.87	Joback Method
cpg	1029.18	J/mol×K	954.73	Joback Method
cpg	1043.31	J/mol×K	988.60	Joback Method
cpg	1056.27	J/mol×K	1022.47	Joback Method
cpg	1068.08	J/mol×K	1056.33	Joback Method
cpg	1078.77	J/mol×K	1090.20	Joback Method

dvisc	0.0004813	Pa×s	520.96	Joback Method
dvisc	0.0002579	Pa×s	581.97	Joback Method
dvisc	0.0001556	Pa×s	642.97	Joback Method
dvisc	0.0001024	Pa×s	703.98	Joback Method
dvisc	0.0000721	Pa×s	764.99	Joback Method
dvisc	0.0000534	Pa×s	825.99	Joback Method
dvisc	0.0000413	Pa×s	887.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4654255&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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