1,3-benzenedicarboxylic acid, diheptyl ester

Inchi: InChI=1S/C22H34O4/c1-3-5-7-9-11-16-25-21(23)19-14-13-15-20(18-19)22(24)26-17-12-
InchiKey: NRVRCDIOAWDMJQ-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCC)c1
Mol. weight [g/mol]: 362.50
CAS: 4654-17-5

Physical Properties

Property code	Value	Unit	Source
af	1.0936		Cheméo Relay (1.0)
hf	-881.99	kJ/mol	Cheméo Relay (1.0)
hfus	51.96	kJ/mol	Joback Method
hvap	99.90	kJ/mol	Cheméo Relay (1.0)
ie	9.19	eV	Cheméo Relay (1.0)
log10ws	-6.62		Cheméo Relay (1.0)
logp	5.941		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
tb	650.97	K	Cheméo Relay (1.0)
tc	847.10	K	Cheméo Relay (1.0)
tf	297.53	K	Cheméo Relay (1.0)
vc	1.186	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4654175&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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