

Terephthalic acid, 4,4-dimethylpent-3-yl octyl ester

Inchi:	InChI=1S/C23H36O4/c1-6-8-9-10-11-12-17-26-21(24)18-13-15-19(16-14-18)22(25)27-20
InchiKey:	GGOGVOQACYKCBY-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCCCCOC(=O)c1ccc(C(=O)OC(CC)C(C)(C)C)cc1
Mol. weight [g/mol]:	376.54

Physical Properties

Property code	Value	Unit	Source
af	1.0129		Cheméo Relay (1.0)
hf	-918.70	kJ/mol	Cheméo Relay (1.0)
hfus	43.62	kJ/mol	Joback Method
hvap	102.92	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.66		Cheméo Relay (1.0)
logp	6.185		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2308.00		NIST Webbook
tb	652.94	K	Cheméo Relay (1.0)
tc	851.07	K	Cheméo Relay (1.0)
tf	324.90	K	Cheméo Relay (1.0)
vc	1.200	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.87	J/mol×K	906.21	Joback Method
cpg	1075.76	J/mol×K	941.10	Joback Method
cpg	1091.37	J/mol×K	975.98	Joback Method
cpg	1105.75	J/mol×K	1010.87	Joback Method
cpg	1118.97	J/mol×K	1045.76	Joback Method
cpg	1131.08	J/mol×K	1080.64	Joback Method
cpg	1142.12	J/mol×K	1115.53	Joback Method
dvisc	0.0004367	Pa×s	519.65	Joback Method
dvisc	0.0002089	Pa×s	584.08	Joback Method

dvisc	0.0001157	Pa×s	648.50	Joback Method
dvisc	0.0000713	Pa×s	712.93	Joback Method
dvisc	0.0000476	Pa×s	777.36	Joback Method
dvisc	0.0000338	Pa×s	841.78	Joback Method
dvisc	0.0000252	Pa×s	906.21	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415971&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

Cheméo Relay (1.0):

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
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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