Terephthalic acid, 4,4-dimethylpent-2-yl heptyl ester

Inchi: InChI=1S/C22H34O4/c1-6-7-8-9-10-15-25-20(23)18-11-13-19(14-12-18)21(24)26-17(2)16-22(3,4)5/h11-14,17H,6-10,15-16H2,1-5H3

InchiKey: DDVGFDJSMYTISK-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OC(C)CC(C)(C)C)cc1

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
af	0.9740		Cheméo Relay (1.0)
hf	-912.59	kJ/mol	Cheméo Relay (1.0)
hfus	41.02	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.32		Cheméo Relay (1.0)
logp	5.795		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
tb	642.57	K	Cheméo Relay (1.0)
tc	835.00	K	Cheméo Relay (1.0)
tf	322.84	K	Cheméo Relay (1.0)
vc	1.157	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.32	J/mol×K	883.33	Joback Method
cpg	1015.05	J/mol×K	917.98	Joback Method
cpg	1030.54	J/mol×K	952.63	Joback Method
cpg	1044.85	J/mol×K	987.28	Joback Method
cpg	1058.01	J/mol×K	1021.93	Joback Method
cpg	1070.07	J/mol×K	1056.58	Joback Method
cpg	1081.10	J/mol×K	1091.23	Joback Method
dvisc	0.0004944	Pa×s	508.38	Joback Method

dvisc	0.0002388	Pa×s	570.87	Joback Method
dvisc	0.0001332	Pa×s	633.36	Joback Method
dvisc	0.0000825	Pa×s	695.86	Joback Method
dvisc	0.0000553	Pa×s	758.35	Joback Method
dvisc	0.0000394	Pa×s	820.84	Joback Method
dvisc	0.0000294	Pa×s	883.33	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=U415955&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

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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