Terephthalic acid, di(6-methylhept-2-yl) ester

Inchi: InChI=1S/C24H38O4/c1-17(2)9-7-11-19(5)27-23(25)21-13-15-22(16-14-21)24(26)28-20(
InchiKey: FVXUWKJHAAAYPJ-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CC(C)CCCC(C)OC(=O)c1ccc(C(=O)OC(C)CCCC(C)C)cc1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-223.62	kJ/mol	Joback Method
hf	-824.35	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.430		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	931.00	K	Joback Method
tc	1143.02	K	Joback Method
tf	483.50	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1121.15	J/mol×K	931.00	Joback Method
cpg	1192.44	J/mol×K	1107.68	Joback Method
cpg	1180.91	J/mol×K	1072.34	Joback Method
cpg	1168.06	J/mol×K	1037.01	Joback Method
cpg	1153.84	J/mol×K	1001.67	Joback Method
cpg	1138.22	J/mol×K	966.34	Joback Method
cpg	1202.67	J/mol×K	1143.02	Joback Method
dvisc	0.0000213	Pa×s	931.00	Joback Method

dvisc	0.0000294	Pa×s	856.42	Joback Method
dvisc	0.0000432	Pa×s	781.83	Joback Method
dvisc	0.0000687	Pa×s	707.25	Joback Method
dvisc	0.0001219	Pa×s	632.67	Joback Method
dvisc	0.0002520	Pa×s	558.08	Joback Method
dvisc	0.0006523	Pa×s	483.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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