1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl heptyl ester

Inchi: InChI=1S/C23H34O4/c1-4-5-6-7-10-13-26-22(24)20-11-8-9-12-21(20)23(25)27-19-15-17

InchiKey: QHTQMYRAFMGSMP-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-215.17	kJ/mol	Joback Method
hf	-760.08	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	88.82	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.529		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
tb	929.74	K	Joback Method
tc	1148.49	K	Joback Method
tf	547.89	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.02	J/mol×K	929.74	Joback Method
cpg	1073.91	J/mol×K	966.20	Joback Method
cpg	1089.14	J/mol×K	1002.66	Joback Method
cpg	1102.74	J/mol×K	1039.12	Joback Method
cpg	1114.73	J/mol×K	1075.58	Joback Method
cpg	1125.14	J/mol×K	1112.03	Joback Method
cpg	1134.00	J/mol×K	1148.49	Joback Method
dvisc	0.0004775	Pa×s	547.89	Joback Method

dvisc	0.0002690	Pa×s	611.53	Joback Method
dvisc	0.0001689	Pa×s	675.17	Joback Method
dvisc	0.0001149	Pa×s	738.82	Joback Method
dvisc	0.0000831	Pa×s	802.46	Joback Method
dvisc	0.0000630	Pa×s	866.10	Joback Method
dvisc	0.0000496	Pa×s	929.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339617&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

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