cis-Cyclohex-4-en-1,2-dicarboxylic acid, heptyl 3-methylbutyl ester

Inchi: InChI=1S/C20H34O4/c1-4-5-6-7-10-14-23-19(21)17-11-8-9-12-18(17)20(22)24-15-13-16

InchiKey: QZQADGKFNCDFKI-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CCCCCCCOC(=O)C1CC=CCC1C(=O)OCCC(C)C

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-306.06	kJ/mol	Joback Method
hf	-859.25	kJ/mol	Joback Method
hfus	43.73	kJ/mol	Joback Method
hvap	78.45	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.672		Crippen Method
mcvol	292.380	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	823.18	K	Joback Method
tc	1020.86	K	Joback Method
tf	448.38	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.11	J/mol×K	823.18	Joback Method
cpg	960.78	J/mol×K	856.13	Joback Method
cpg	978.14	J/mol×K	889.07	Joback Method
cpg	994.20	J/mol×K	922.02	Joback Method
cpg	1008.98	J/mol×K	954.96	Joback Method
cpg	1022.51	J/mol×K	987.91	Joback Method
cpg	1034.79	J/mol×K	1020.86	Joback Method
dvisc	0.0011375	Pa×s	448.38	Joback Method

dvisc	0.0005375	Pa×s	510.85	Joback Method
dvisc	0.0002991	Pa×s	573.31	Joback Method
dvisc	0.0001867	Pa×s	635.78	Joback Method
dvisc	0.0001268	Pa×s	698.25	Joback Method
dvisc	0.0000918	Pa×s	760.71	Joback Method
dvisc	0.0000698	Pa×s	823.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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