

1,2-Cyclohexanedicarboxylic acid, cyclobutyl heptyl ester

Inchi:	InChI=1S/C19H32O4/c1-2-3-4-5-8-14-22-18(20)16-12-6-7-13-17(16)19(21)23-15-10-9-1
InchiKey:	LENZWEPFXDUECM-UHFFFAOYSA-N
Formula:	C19H32O4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCC1
Mol. weight [g/mol]:	324.45

Physical Properties

Property code	Value	Unit	Source
gf	-293.35	kJ/mol	Joback Method
hf	-824.47	kJ/mol	Joback Method
hfus	39.48	kJ/mol	Joback Method
hvap	76.41	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.402		Crippen Method
mcvol	271.730	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	2257.00		NIST Webbook
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tb	812.59	K	Joback Method
tc	1018.87	K	Joback Method
tf	465.77	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.32	J/molxK	812.59	Joback Method
cpg	981.86	J/molxK	984.49	Joback Method
cpg	967.65	J/molxK	950.11	Joback Method
cpg	952.12	J/molxK	915.73	Joback Method
cpg	935.25	J/molxK	881.35	Joback Method
cpg	916.99	J/molxK	846.97	Joback Method
cpg	994.78	J/molxK	1018.87	Joback Method
dvisc	0.0001713	Paxs	812.59	Joback Method

dvisc	0.0002150	Paxs	754.79	Joback Method
dvisc	0.0002802	Paxs	696.98	Joback Method
dvisc	0.0003831	Paxs	639.18	Joback Method
dvisc	0.0005574	Paxs	581.38	Joback Method
dvisc	0.0008809	Paxs	523.57	Joback Method
dvisc	0.0015597	Paxs	465.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U339753&Units=SI

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

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