

1,2-Cyclohexanedicarboxylic acid, 2-ethoxyethyl heptyl ester

Inchi:	InChI=1S/C19H34O5/c1-3-5-6-7-10-13-23-18(20)16-11-8-9-12-17(16)19(21)24-15-14-22
InchiKey:	OIDSXNAENNBEBN-UHFFFAOYSA-N
Formula:	C19H34O5
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC
Mol. weight [g/mol]:	342.47

Physical Properties

Property code	Value	Unit	Source
gf	-447.00	kJ/mol	Joback Method
hf	-1023.33	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	78.73	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.886		Crippen Method
mvol	288.460	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
tb	824.00	K	Joback Method
tc	1019.70	K	Joback Method
tf	473.58	K	Joback Method
vc	1.097	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.27	J/molxK	824.00	Joback Method
cpg	958.87	J/molxK	856.62	Joback Method
cpg	976.14	J/molxK	889.23	Joback Method
cpg	992.07	J/molxK	921.85	Joback Method
cpg	1006.67	J/molxK	954.47	Joback Method
cpg	1019.94	J/molxK	987.08	Joback Method
cpg	1031.88	J/molxK	1019.70	Joback Method
dvisc	0.0007793	Paxs	473.58	Joback Method

dvisc	0.0004039	Paxs	531.98	Joback Method
dvisc	0.0002384	Paxs	590.39	Joback Method
dvisc	0.0001548	Paxs	648.79	Joback Method
dvisc	0.0001079	Paxs	707.19	Joback Method
dvisc	0.0000795	Paxs	765.60	Joback Method
dvisc	0.0000611	Paxs	824.00	Joback Method

Sources

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=U339909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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