Pimelic acid, isobutyl 2-(2-methoxyethyl)hexyl ester

Inchi: InChI=1S/C20H38O5/c1-5-6-10-18(13-14-23-4)16-25-20(22)12-9-7-8-11-19(21)24-15-17

InchiKey: BPYZGLLTOYKPSH-UHFFFAOYSA-N

Formula: C20H38O5

SMILES: CCCCC(CCOC)COC(=O)CCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-460.20	kJ/mol	Joback Method
hf	-1088.51	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.522		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	2326.00		NIST Webbook
rinpol	2326.00		NIST Webbook
tb	831.12	K	Joback Method
tc	1019.53	K	Joback Method
tf	451.71	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.80	J/mol×K	831.12	Joback Method
cpg	1080.94	J/mol×K	988.13	Joback Method
cpg	1067.40	J/mol×K	956.73	Joback Method
cpg	1052.72	J/mol×K	925.33	Joback Method
cpg	1036.90	J/mol×K	893.92	Joback Method
cpg	1019.93	J/mol×K	862.52	Joback Method
cpg	1093.35	J/mol×K	1019.53	Joback Method
dvisc	0.0000335	Pa×s	831.12	Joback Method

dvisc	0.0000456	Pa×s	767.88	Joback Method
dvisc	0.0000658	Pa×s	704.65	Joback Method
dvisc	0.0001019	Pa×s	641.41	Joback Method
dvisc	0.0001737	Pa×s	578.18	Joback Method
dvisc	0.0003376	Pa×s	514.95	Joback Method
dvisc	0.0007901	Pa×s	451.71	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=U406743&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