

Pimelic acid, butyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H36O4/c1-6-7-13-22-17(20)11-9-8-10-12-18(21)23-15-16(2)14-19(3,4)5/h1
InchiKey: SGVKLWRQFDKCPH-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-358.34	kJ/mol	Joback Method
hf	-939.12	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.896		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	783.03	K	Joback Method
tc	968.31	K	Joback Method
tf	435.63	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.66	J/molxK	783.03	Joback Method
cpg	928.69	J/molxK	813.91	Joback Method
cpg	945.69	J/molxK	844.79	Joback Method
cpg	961.70	J/molxK	875.67	Joback Method
cpg	976.73	J/molxK	906.55	Joback Method
cpg	990.82	J/molxK	937.43	Joback Method
cpg	1004.00	J/molxK	968.31	Joback Method
dvisc	0.0010903	Paxs	435.63	Joback Method

dvisc	0.0004713	Paxs	493.53	Joback Method
dvisc	0.0002430	Paxs	551.43	Joback Method
dvisc	0.0001421	Paxs	609.33	Joback Method
dvisc	0.0000912	Paxs	667.23	Joback Method
dvisc	0.0000628	Paxs	725.13	Joback Method
dvisc	0.0000457	Paxs	783.03	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=U406470&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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