Terephthalic acid, isohexyl 2-heptyl ester

Inchi: InChI=1S/C21H32O4/c1-5-6-7-10-17(4)25-21(23)19-13-11-18(12-14-19)20(22)24-15-8-9
InchiKey: FASQCLDNTAMBBL-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCC(C)OC(=O)c1ccc(C(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-244.00	kJ/mol	Joback Method
hf	-751.87	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.405		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	2446.00		NIST Webbook
tb	863.24	K	Joback Method
tc	1067.43	K	Joback Method
tf	479.69	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.15	J/mol×K	863.24	Joback Method
cpg	954.70	J/mol×K	897.27	Joback Method
cpg	970.02	J/mol×K	931.30	Joback Method
cpg	984.13	J/mol×K	965.34	Joback Method
cpg	997.06	J/mol×K	999.37	Joback Method
cpg	1008.83	J/mol×K	1033.40	Joback Method
cpg	1019.48	J/mol×K	1067.43	Joback Method
dvisc	0.0006933	Pa×s	479.69	Joback Method
dvisc	0.0003257	Pa×s	543.62	Joback Method

dvisc	0.0001793	Pa×s	607.54	Joback Method
dvisc	0.0001106	Pa×s	671.47	Joback Method
dvisc	0.0000742	Pa×s	735.39	Joback Method
dvisc	0.0000531	Pa×s	799.32	Joback Method
dvisc	0.0000399	Pa×s	863.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U356290&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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